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NATIONAL BUREAU OF STANDARDS REPORT

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PRELIMINARY REPORT
ON THE THERMODYNAMIC PROPERTIES OF
SELECTED LIGHT-ELEMENT AND
SOME RELATED COMPOUNDS

(Supplement to NBS Reports 6297, 6484, 6645, 6928, 7093, 7192, 7437, 7587, 7796, 8033, and 8186)

1 July 1964

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U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

Mary A. Kuvanec

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Twelfth Technical Summary Report
to the Advanced Research Projects Agency
on the Thermodynamic Properties
of Light-Element Compounds

Reference: ARPA Order No. 20

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ABSTRACT

This is the twelfth semiannual report on the current experimental, theoretical, and evaluative program, at the National Bureau of Standards, on the thermodynamic properties of selected light-element and some related compounds of primary interest in high-temperature research. Included are detailed surveys of accomplishments during the past year and program plans for the next; new experimental results in several areas; literature surveys and critical data evaluations; and tables of thermodynamic functions and heats of formation.

The microwave transitions of $A\ell F$ and $A\ell C\ell$ were observed at elevated temperatures, and were analyzed to give certain molecular constants. Rough estimations of the experimental vapor concentrations are in agreement with the current values for the dissociation energies. A new cell for phase purifications and thermal analyses (such as of BeF_2) was constructed and is described in detail. The studies on the kinetics of evaporation of $A\ell_2O_3$ continued with attention to the steady-state conditions of heat flow and evaporation. Preliminary mass-spectrometric results on a new molecule, $BeOA\ell$, are described, and its molecular constants were estimated by analogy. Thermodynamic parameters were computed for an aluminum wire exploding in an air environment, and, with critical discussion, are presented graphically and tabularly from 1500° to 6000°K and from 0.01 to 1000 atm. pressure.

Largely as a result of experimental work elsewhere, improved values are given for the heats of formation of crystalline $A\ell_4C_3$, LiF, BeF_2, $A\ell F_3$, and MgF_2. New molecular constants for the BeF_2 molecule create excellent thermodynamic consistency for the mass-spectrometric data reported earlier for the new molecule Be_2OF_2. A literature survey was made of the existing heat-capacity and relative-enthalpy data of approximately 70 compounds of Ba, Ca, Cr, Fe, K, and Si.

Numerous tables are presented in four appendices. These include a table of up-to-date critical values of physical constants important in thermodynamic work. Tables of ideal-gas thermodynamic functions were computed and are given for H^-, O^-, F^-, $C\ell^-$, N_2^+, O_2^+, NO^+, nine neutral diatomic hydrides, LiO, BeF_2 (revised), and $BeOA\ell$. As the result of a current revision of NBS Circular 500 (Series I), tentative new values are given for numerous primitive compounds of O, H, the halogens, S, Se, Te, N, P, B, and C. Also given is a preliminary list of ionization potentials and electron affinities of over 190 light-element atoms and molecules, together with estimated errors in most cases.

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PART A. SUMMARY OF RESEARCH ACCOMPLISHMENTS AND PLANS FOR FUTURE WORK

INTRODUCTION

When more than ten years ago chemical propulsion became a subject of major practical importance, the dearth of available thermodynamic information on compounds of the light elements, particularly the more metallic ones, became apparent. Since that time a large number of laboratories, in this country as well as abroad, has filled an impressive number of data gaps in this area, though work still remains to be done in confirming or revising old values and in determining new ones hitherto uninvestigated.

Earlier research programs at the National Bureau of Standards, notably those on boron compounds and on the calculation of thermodynamic properties of common gases to high temperatures, have made contributions of material importance in this field, while other groups oriented to different primary aims continue to supply valuable information. The current NBS program, involving many groups systematically studying the thermodynamic properties of light elements primarily to fill propulsion needs, began in 1958, and since then has issued reports similar to the present one at six-month intervals, as indicated by the report numbers on the title page. This current NBS program continues to deal largely with those simple compounds, such as of beryllium and aluminum, which are of some importance as high-temperature combustion products.

In Part A of this report is given a rather detailed account of what each NBS group in the program has accomplished during the past year, and what it plans to accomplish during the next fifteen months. In many cases detailed descriptions of apparatus and methods being used were given in earlier reports, and are omitted here except for reference to modifications and improvements. Complete descriptions and experimental results are to be found in earlier reports of this series and in Part B of the present report, or are deferred to future reports in the interest of less preliminary and less fragmentary accounts.

These NBS "Preliminary Reports" have included not only new results, but also literature coverages, critical assessments in certain categories, and thermodynamic tables. It is evident that in so fast developing a field many of these presentations, if once up-to-date, are no longer so. One important objective of the program is to bring up-to-date all past reports, and it is anticipated that, through systematic effort, a substantial amount of this work will have been accomplished within the next fifteen months.

1. LIGHT-ELEMENT EQUATION OF STATE
EXPLODING WIRE PROGRAM

The exploding wire project is an experimental program which was undertaken in order to develop a system suitable for direct experimental measurement of thermodynamic quantities under high-temperature (above 2,000° K), high-pressure (up to 100 atm) conditions. Because of the transient nature of the experiments, considerable study and development work on the techniques of fast-measurement have been and continue to be a necessary and major part of the program. For example, techniques of fast-measurement are required for each of the following:

1.) For electrical measurements (of current and voltage in a transient electrical discharge);

2.) For velocity measurements (by optical and x-ray methods);

3.) For temperature measurements (by time-resolved spectrographic and pyrometric methods);

4.) For dynamic pressure measurements;

5.) For time-resolved photographic observations, etc.

The program also requires theoretical studies of the thermodynamic and hydrodynamic behavior of the exploding wire system. These studies approximate the experimental conditions, and the results serve to guide the experimental program. All of this work will continue during the next fiscal year.

Activity Summary - July 1, 1963 to June 30, 1964

The work for this fiscal year has been devoted to the tasks discussed in the following paragraphs.

1.) Electrical Energy Measurements. The task of measuring the energy dissipated in a given sample during a transient electrical discharge, where the resistance of the sample is a variable, continues to be a major problem. A number of calibration experiments, in which a calorimeter tube (a tube of known and fixed resistance) was inserted in the discharge circuit in place of the sample, have shown agree-

The high-speed framing and drum camera and the photomultiplier records from these experiments show in some detail the hydrodynamic behavior of the wire vapor as it expands and mixes with the surrounding air. The records indicate the time interval (during the explosion) and the place (in the vessel) where the conditions of thermodynamic equilibrium, which are essential for meaningful spectroscopic studies, can be expected to exist. A few more experiments using time-resolved, pulse x-ray techniques are required to complete this part of the work.

However, to date the experiments seem to indicate that the temperature distribution is uniform throughout the mixture for nearly 0.5 msec, and that it is during this interval that one could expect a series of conditions of thermodynamic equilibrium to prevail.

The spectroscopic records from these preliminary experiments show emission spectra from Al atoms and AlO molecules. There was no evidence of bands or lines from the air components. However, it is expected that spectra from these latter components will appear when the electrical energy input to the wire is increased. A 20 kv, 60 μf capacitor bank has now been constructed for this purpose. Further, a six-channel photomultiplier system for viewing the spectra has been designed and is now being adjusted. This system will be used to make time-resolved observations of the intensities of individual spectral lines during the explosion. From these data it is anticipated that one may determine the temperature of the mixture and the relative concentrations of atoms, molecules, and ions in the mixture.

3.) Thermodynamic Calculations. A series of thermodynamic calculations has been performed for the aluminum-air gas mixture generated by the explosion of a wire such as that described in paragraph 2. The results of these calculations, which enable one to estimate the energy requirements for and the relative concentrations of the various components in a given temperature-pressure region, are given in Chapter B-3 in this report. A general-purpose computer program for making such thermodynamic calculations was prepared for this work. This program is intended for use in future calculations with different mixtures.

ment (to better than 2 %) between the heat energy ($m\ c\ \Delta T$) and the energy as determined from measurement of the discharge current (i.e. from $\int I^2 R\ dt$ where I is the current and R is the constant resistance of the calorimeter tube). However, these same experiments have shown large disagreement (10 to 30 %) between $m\ c\ \Delta T$ and the energy as determined from simultaneous measurement of the transient current and voltage ($\int E\ I\ dt$ where E is the voltage measured across the calorimeter tube). Proper determination of E is, of course, required for measurement of energy dissipation in cases where the sample is melted or vaporized by the discharge.

More recent experiments, with discharge voltages again in the range from 5 to 10 kv and ringing frequencies of approximately 12 kc, indicate that considerable errors are introduced in the voltage measurements by ground currents in the measuring system and by sizeable changes in the main circuit resistance due to the skin effect. These errors are now being minimized and, if necessary, corrections will be applied to compensate for the errors.

At the higher voltages (up to 100 kv) and frequencies (up to 300 kc) which will be used for very rapid pulsing of the sample, the measurement of voltage and current becomes increasingly difficult. To meet these difficulties, a technique, which employs an adjustable compensating coil for experimentally removing erroneous induced voltages, from the measurements, has been devised and is now being used for a series of experiments.

It is expected that the effort required for making energy measurements will be greatly reduced by the use of a new system for automatic scanning and recording of the transient voltage and current curves. This system is now being tested for accuracy.

2.) Temperature and Concentration Measurements.

The initial task of this phase of the program which was initiated in this fiscal year, has been the design and construction of an exploding wire system suitable for spectroscopic studies. A small 20 kv, 15 μf system was constructed and used for a series of preliminary exploratory experiments, in which aluminum wires (0.1 mm in diameter) were exploded in a closed vessel containing air at normal pressures. During these preliminary experiments, time-resolved photographic and photoelectric observations of the entire explosion process were conducted. The integrated light from the entire explosion was also observed spectrographically.

2. LOW-TEMPERATURE CALORIMETRY

Objectives

Accurate measurements of the heat capacity are made between 15° and 400°K and the thermal functions calculated from the data. Survey and analysis of the literature data on substances of interest are conducted complementing the above work. Computer codes are developed for processing the experimental and literature data. Where data are unavailable or inadequate, efforts are made to obtain pure samples for experimental investigations.

Activity Summary - July 1, 1963 to June 30, 1964

Heat-capacity measurements on chrysoberyl ($BeO \cdot Al_2O_3$) were completed and a paper on the results is now undergoing editorial review. Comparison of the heat capacity of $BeO \cdot Al_2O_3$ with that of an equimolar mixture of BeO and Al_2O_3 showed the heat capacity of chrysoberyl to be about 1 percent higher from about 200° to 400°K. Below about 200°K, the heat capacity of chrysoberyl deviates positively with decrease in temperature, being about 28 percent higher at 10°K. The investigation of the additivity of heat capacity of other "mixed-oxides" compounds revealed similar increase in positive deviation with decrease in temperature.

A paper combining the low- and high-temperature heat measurements on aluminum carbide (Al_4C_3) was prepared. The results are compared in conjunction with heat of formation of Al_4C_3 obtained by another group in the program, with extensive vapor-equilibrium data available in the literature involving Al_4C_3. Considerable deviation is shown between the vapor pressure calculated from thermal data and those experimentally observed. The paper has undergone editorial review, but a recent revision of the heat of formation of Al_4C_3 (See Chapter B-1 of this report) necessitates recalculation of the comparison of vapor-equilibrium data.

The literature data on $LiBH_4$, NaF, NaCl, $NaBH_4$, KF, KCl, KBr, and KBH_4 and unpublished data on BeF_2 were analyzed and thermal functions calculated. Tables were given in NBS Report 8186, which is dated 1 January 1964.

Plans for the Period July 1, 1964 to September 30, 1965

Heat-capacity measurements on $BeO \cdot 3Al_2O_3$, BeF_2, Li_2BeF_4, Li_3AlF_6, and BeO are planned. Samples of the above substances, except BeF_2, are on hand. A highly pure sample of BeF_2 is being prepared by another group in the program. The crystallites of the above sample of BeO are considerably larger than those previously investigated. The new measurements should yield information on the relative size effect on the heat capacity.

Literature analysis of heat-capacity data on mixed oxides, halides, and oxyhalides of Aℓ, Be, Fe, Cr, Si, Ca, Ba, and K will be conducted.

3. HIGH-TEMPERATURE CALORIMETRY

This work includes all enthalpy measurements (giving also heat capacities, relative entropies, and heats of fusion and transition) from approximately room temperature to 2800°K. The "drop" method is used exclusively, in the sense that a sample at a known fixed temperature is transferred rapidly to a calorimeter operating near room temperature.

The following three apparatuses are available:

1. A silver-core resistance-heated furnace and an ice calorimeter. This apparatus has been in use for many years. The available temperature range is 273° to approximately 1200°K.

2. A platinum-containing resistance-heated furnace and an ice calorimeter. The available temperature range is 273° to approximately 1800°K.

3. An induction-heated furnace and an adiabatic calorimeter. The available temperature range is 1200° to 2800°K.

During the past year enthalpy measurements were carried out on $Li_3A\ell F_6$ in the solid range (273° to 973°K), and on a second (purer) sample of $BeO \cdot A\ell_2O_3$ (273° to 1173°K). Chemical analyses were completed on the sample of Li_2BeF_4 whose enthalpy had been measured earlier (273° to 873°K), permitting precise thermal corrections to be made for the deviation from the nominal stoichiometric composition. The detailed results on those three substances were given in the last semiannual report (NBS Report 8186, 1 January 1964, pp. 62-82). These data were obtained using the first apparatus mentioned above. The apparatus is being overhauled, as special tests indicate a substantially poorer precision than earlier, though still as high an absolute accuracy as is possible with the reduced precision.

Plans for the Next 15 Months

Using the first apparatus, some new measurements on $BeO \cdot A\ell_2O_3$ will be undertaken in an effort to improve on the accuracy of the earlier data for this substance. (A sample of pure $BeO \cdot 3A\ell_2O_3$ also is available, and this may be measured too.) Measurements on $Li_3A\ell F_6$ will be extended into the liquid range (up to 1200°K). In addition, another NBS group is attempting to prepare one or more pure polymorphs of BeF_2, and if such samples become available, enthalpy measurements will be undertaken to well into the liquid range. The derivation of the heat of fusion of BeF_2 from the data will depend, however, on the ability of the fluorine-calorimetry group to make suitable measurements of the heat of solution of the sample quenched in the drop calorimeter, for comparison with the heat of solution of one or more well-defined crystalline polymorphic forms.

Measurements on graphite and various preliminary tests with the third apparatus mentioned above (for enthalpy measurements from 1200°K to 2800°K) have indicated several minor modifications to improve precision and accuracy and to facilitate the experimental work. When these modifications are made, measurements will be undertaken on alpha aluminum oxide ($A\ell_2O_3$) from about 1200°K to the highest temperature the capsule material will withstand. These data should include the heat of fusion and the heat capacity of the liquid.

4. FLUORINE COMBUSTION CALORIMETRY: REACTION CALORIMETRY OF FLUORINE AND FLUORIDES

Background and Current Studies

During the initial stages of the contract now under way a procedure was developed for determining the energy of combustion in fluorine of metals forming fluorides of low volatility, and hence determining the enthalpy of formation of the solid fluoride. The procedure involves the combustion of a pellet prepared from the finely granulated metal mixed with Teflon, which aids ignition and causes the reaction to continue to near completion.

Using the method described above, the enthalpy of formation of crystalline aluminum fluoride was determined, as well as the enthalpy of combustion of Teflon in fluorine. The method is now being applied to the combustion of beryllium.

At the time we undertook these studies we realized that beryllium was a very refractory metal on the basis of a similar series of experiments attempted at the Atlantic Research Corporation. Just how refractory it was we did not fully realize and at the time we undertook the measurements we thought that we had an experimental procedure which should resolve the difficulties entailed by the refractory character of the metal. The results of the measurements with beryllium, however, indicate that this procedure is inadequate to obtain complete combustion of beryllium in fluorine and that the Teflon pelleting procedure is not an infallible method of obtaining complete combustion of a refractory metal. Nevertheless we feel that the results of our experiments so far are of sufficient interest to be described here.

In our efforts to achieve more nearly complete combustion we have used increased pressure of fluorine, and we have attempted to isolate the reaction zone and modify the construction of the supports to allow a higher reaction temperature. The upper limit of fluorine pressure that we have used is 21 atm. In attempting to achieve higher reaction temperatures we have used supports with lower thermal contact with the bomb body and less massive metal supports. The limits of this method of approach were reached in one experiment in which the combustion of the sample resulted in ignition of the stainless steel sample support and a fire in the bomb which lasted until the fluorine was completely gone. The severe damage to the bomb parts was sufficient to restrain us from further experiments in this direction. With metal supports the maximum combustion is in the range of 80 to 90 percent. We have also attempted to use ceramic supports for the sample. Experiments using calcium fluoride have led to the highest percent combustion thus far achieved, somewhat greater than 90 percent. The use of magnesium fluoride will also be explored. We feel that our experiments have reached a point from which we must continue using the procedures which we have thus far developed. We shall use combustions on metal supports and on ceramic support to substantiate one another.

Determination of the amount of reaction is a major problem in this as in all novel reaction procedures. In this case it is accentuated by the incompleteness of the reaction.

To determine the amount of unburned material at the conclusion of a combustion we have adopted a procedure of dissolving the residue in alkali or acid and measuring evolved hydrogen. At present we are using a strong alkali solution. The hydrogen evolved is collected by a Toepler pump and its volume is measured. The sensitivity of this method is approximately 0.01 milligram of beryllium. The accuracy is approximately .03 to .05 mg of beryllium. When a 100 milligram sample of beryllium is used this is adequate.

The purity of the starting material is another factor in determining the amount of reaction. The beryllium we are using is a powder 100 mesh or smaller which we obtained from Nuclear Metals Inc. Impurities of metal and carbon amount to less than 0.02 percent. However, oxygen impurity is 0.18 percent as determined by neutron activation analysis. Our experience with beryllium and our previous experience with aluminum indicate that oxygen can be a significant impurity even in metal having very small amounts of other impurities.

In the preparation of the beryllium-Teflon pellet we have been at some pains to prevent loss of weight. The most successful procedure so far is the formation of a mixture of the powder in a Teflon filled bag. The bag and enclosed mixture are then pelleted together. While somewhat cumbersome, this method has been shown to reduce losses of weight on formation of the pellet to an almost negligible amount. Typical parameters are a 0.05 gram bag, 2 to 2.2 grams of Teflon powder, and 100 milligrams of beryllium. In the preparation of pellets weight losses range from 0 to 0.1 mg. On combustion, the Teflon supplies approximately 27 kJ, the beryllium supplies 10 to 12 kJ. Energy from the tungsten fuse amounts to approximately 20 J.

Characterization of the combustion products is also an important factor. The beryllium fluoride formed in the combustion is in a glassy form of which most is deposited on the walls of the bomb as a fine dust. This has accentuated handling problems on account of the toxicity of the dust, and in order to handle the material safely we carry out all bomb loading and unloading processes in a dust box. Although the work recently described by Dr. A. R. Taylor Jr. will be of value to us, we feel that it will be necessary for us also to determine the heats of solution of the beryllium fluoride dust formed in our experiment. This is because we have no reason to assume that the energy state of the very fine dust which we obtain is the same as that of the rather massive glassy material which Dr. Taylor used in his experiments. Our measurements on the dust formed in our experiment and on crystalline beryllium fluoride obtained in other work at the National Bureau of Standards will allow us to refer our measurements directly to the heat of formation of crystalline beryllium fluoride.

In addition to the solution calorimetry associated with the heat of formation of BeF_2, an additional calorimetric study is being made of the formation of Li_2BeF_4 from LiF and BeF_2. In this work preliminary studies of the solubilities of the materials have been made, to find a suitable solvent. Undertaking the study of the three substances LiF, BeF_2 and Li_2BeF_4 introduces limitations on the solvent that can be used, as it would be desirable to determine the enthalpy of solution in such a solvent that the final solution is the same in every case. By this means dilution effects and problems of ionic strength and ionic interactions can be avoided. A suitable solvent is aqueous $HC\ell$, with LiF or BeF_2 added in some cases. Studies under way but not completed include attempts to find a suitable container. Glass can be used, but because of its interaction with HF formed by hydrolysis of the salts in a solution of a strong acid, a correction would be necessary for the glass dissolved. The magnitude of this correction has been estimated.

In addition to the studies on solid fluorides, one study has been made of the enthalpy of formation of aluminum carbide ($A\ell_4C_3$) by combustion in oxygen. Combustion procedures leading to complete combustion in a calorimeter bomb were developed. A significant finding of the study was the demonstration that under the conditions of the bomb combustion, a large fraction of the aluminum was converted to the little known delta phase of aluminum oxide. The delta phase is formed when gaseous aluminum oxide, in the presence of nitrogen and carbon dioxide, condenses on the cold surfaces of the bomb. The energy difference between delta- and alpha-aluminum oxide was determined in another laboratory from measurements on the combustion products obtained in the experiments.

Within the past year we have begun to reconstruct a flame calorimeter for combustion of gases in fluorine or combustion of fluorine containing gases. This effort is particularly directed to a study of the heat of formation of F_2O, which is now readily available in substantial quantities and in a moderately high degree of purity.

Plans for continuation

All work necessary to establish the energy of combustion of beryllium in fluorine, and such solution calorimetry as is necessary to establish the heat of formation of both glassy and crystalline BeF_2, will be completed. The solution calorimetry of Li_2BeF_4 will also be completed following the general procedure described above.

In the flame calorimeter the study of OF_2 will be completed and a study will be made of $C\ell F_3$.

The literature of the fluorine compounds will be used to prepare summaries of best values, revised to include recent work, and other summaries useful in future resumes of the thermodynamic properties of fluorine compounds.

5. LIGHT ELEMENT COMPOUNDS

1. Summary for Fiscal Year 1964

A great deal of effort has been spent this year in studying aluminum borohydride. A heat of formation value on this material is of first importance. Two samples have been obtained from the Union Carbide Chemicals Corporation, but only the earlier one has been studied by our group.

An apparatus for the purification of aluminum borohydride by successive distillation has been constructed. This apparatus incorporates means of measuring volumes, pressures, and densities. It is a vacuum-line type of apparatus controlled largely by mercury valves to prevent reaction, and subsequent contamination with stopcock grease.

Many experiments have been run on hydrolysis of this material using water, dilute sulfuric acid, and whole series of alcohols. This involved various methods of contacting the aluminum borohydride with the reagents. Some methods differed in mechanical design of apparatus. Others involved the order of addition of solvents or the liquid or vapor contact. Apparently the most successful method was contacting the aluminum borohydride vapor with isopropyl alcohol vapor followed by 2N sulfuric acid to complete the hydrolysis. Even this method failed to give good stoichiometric results.

Aluminum borohydride is quite sensitive to heat, forming the rather inert mixtures of aluminum borides in small quantities. For this reason the hydrolysis must be very gentle.

When it became known that the aluminum borohydride contained some hydrocarbon, a capillary gas chromatograph was modified to attempt to separate the relatively small amounts of hydrocarbon from larger amounts of hydrogen. This work is still in progress.

Work has continued on the mass spectra of gases issuing from the Knudsen Cell containing a light-element hydride. A great many m/e peaks can be explained but any quantitative treatment leaves many unexplained residues. Apparently this is much the same problem as would be encountered by heating an organic polymer in the cell. This study has been recessed temporarily.

The literature study on light-element oxides and hydrides, and alloys and intermetallic compounds was continued.

In the fiscal year 1964, new apparatus and techniques were developed for the preparation of pure polymorphic crystalline forms of BeF_2. A special cell for phase purifications and thermal analyses to 1000°C has been completed by our shops. This cell is designed for a large number of different types of phase purifications with BeF_2 such as distillation, sublimation, crystallization and preferential decomposition. The capacity of the cell is such that sizeable quantities (about 50 grams) of material may be processed at one time.

The platinum parts (rupture-disc ampoule, cup and support) have been secured for the hydrofluorothermal growths of the beta quartz-like form of BeF_2 in a bomb under a high pressure of HF. The technique of anhydrous addition of HF in the closed ampoule is nearing perfection.

2. Plans for Period July 1, 1964 to September 30, 1965

The project will furnish analytical, preparative, and purification support to the thermochemical groups engaged in the program. The present problem is the method of hydrolysis and analysis of aluminum borohydride. In the event that the material received needs some purification this may also be undertaken. The general analytical or purification work will be assigned to personnel best qualified to handle the particular work. The literature survey of oxides and hydrides and of alloys and intermetallic compounds will be continued.

The phase purification and thermal analysis cell will be used for the preparation of pure polymorphic crystalline forms of BeF_2 by a large number of different types of phase purifications. The procedures yielding pure polymorphs will be used to obtain sufficient material for the Bureau needs for establishing the thermodynamic and related properties of BeF_2. The hydrofluorothermal process will also be used to obtain smaller amounts of the beta quartz-like form of BeF_2.

Upon completion of the above, effort will be directed towards the establishment of the phase diagrams to 1000°C of the trielement systems Be-B-O, Al-B-O, Be-B-F and Al-B-F, and the preparation in pure crystalline form of any compounds existing in these systems up to 1000°C.

6. HALIDE SOLID-VAPOR EQUILIBRIA (TRANSPIRATION METHOD)

Following the series of precise measurements of the vapor pressure of solid AlF_3 from 1233° to 1288°K mentioned in an earlier report (NBS Report 8033, 1 July 1963, p. 10), the transpiration apparatus was adapted to allow introducing $AlCl_3$ vapor into the argon carrier gas (by evaporating the solid chloride in a boiling-liquid thermostat) and to provide for determining the transpired $AlCl_3$ (by condensation in a weighable cold trap).

Two preliminary runs on the mixed system, with the $AlCl_3$ evaporated at about 373°K and the AlF_3 evaporated at about 1250°K, showed about 66% more AlF_3 evaporated than if the $AlCl_3$ had not been present. The partial pressures of the $AlCl_3$ and AlF_3 have not yet been varied in the usual way that will help define the reaction or reactions taking place. Conceivably, substantial amounts of mixed dimers may have resulted, and this possibility has not yet been explored. It appears more likely, however, that under the conditions of the measurements the gaseous reactions are mainly

$$AlF_3 + (1/2)AlCl_3 = (3/2)AlF_2Cl \qquad (1)$$

and

$$AlF_3 + 2AlCl_3 = 3AlFCl_2 \ . \qquad (2)$$

But the total amount of $AlCl_3$ present was entirely insufficient according to reaction (2), and just barely sufficient according to reaction (1), to explain the observed amount of reacting AlF_3. It is thus tentatively concluded from these preliminary experiments that most of the product was probably AlF_2Cl and that little of it could have been $AlFCl_2$. On the basis of reaction (1) only, the few observed results correspond to a slightly exothermic reaction, in contrast to several estimates made elsewhere.

Unfortunately, owing to the highly reactive nature of $AlCl_3$ some contamination occurred. This has been largely eliminated by replacing or gold-plating all nickel parts of the hot train, by substituting liquid-nitrogen-dried helium for the carrier gas, and by more rigorous out-gassing, but some remaining deficiency in the amount of $AlCl_3$ recovered will necessitate tests for its possible entrapment in the reactive zone of the furnace.

During the coming months the investigation of the $A\ell F_3$-$A\ell C\ell_3$ system will continue, with variation in partial pressures and temperature to define the occurring reactions and check their heats. Subsequent extension to the $A\ell F_3$-HF system in a search for the formation of gaseous Aℓ-H-F species is planned.

7. HIGH-TEMPERATURE MICROWAVE SPECTROSCOPY

During the past year microwave measurements on AℓF and AℓCℓ have been completed. Accurate values of the rotational constants, rotation-vibration interaction constants, electric dipole moments, and nuclear quadrupole coupling constants have been obtained for both molecules. The nuclear quadrupole hyperfine structure in AℓCℓ was extremely complex, but improvements in the spectrometer resolution have led to a satisfactory analysis.

Microwave work on the alkali hydroxides and metaborates has been less successful. Intensive efforts to detect the spectra of NaOH and KOH have so far met with failure. The reason for this is not clear. Although some decomposition probably takes place under the operating conditions which were used, we feel that a reasonable amount of hydroxide vapor was present in the absorption cell. The most likely explanation for the failure to observe spectra is the presence of a large fraction of dimer, which would show no microwave absorption.

Plans for the next year include possible further attempts to detect the alkali hydroxide spectra if suitable changes in conditions can be achieved. A search will also be made for microwave spectra of $A\ell F_2$ and $A\ell C\ell_2$ under conditions similar to those used in the studies of AℓF and AℓCℓ. Microwave investigations of certain interhalogen compounds and nitrogen-fluorine compounds are also planned. In addition, we plan to carry out infrared studies on aluminum borohydride, and possibly on beryllium borohydride, in order to obtain a reliable vibrational assignment.

8. VAPORIZATION OF REFRACTORY SUBSTANCES

(A) ARC-IMAGE RESEARCH

The quadrupole mass filter did not arrive as expected during the past year, but work has continued in the following areas: preliminary temperature measurements with recording automatic optical pyrometer, quantitative measurement of vaporization rates of liquid alumina in 1 atm. of Ar or water vapor, modification of system for use of partial pressures of ambient gas at less than 1 atm. and determination of the temperature of liquid alumina in vacuum and in convective conditions.

Theoretical calculations of expected vaporization rates in Ar, He and Ne suggested the requirement of static gaseous environments, and analysis of the uncertainty in vaporization rates obtained in 1 atm. of static Ar indicated the need to operate at lower partial pressures. Preliminary determination of temperature of the liquid alumina indicated that the molten portion of the sample was heated above the melting point and that a steady-state flow of heat existed across the liquid-solid interface.

Initial observations indicate difficulty in melting MgO with the arc-image furnace due to high sublimation pressure and condensation on the flask.

Projected Plans: July 1, 1964 - October 1, 1965

The following research intended for the next fifteen months with the arc-image furnace:

1. Completion of theoretical and quantitative investigation on vaporization of molten $A\ell_2O_3$ in Ar, He, Ne, H_2, O_2 and H_2O; qualitative observations of molten BeO in these gases and vacuum.

2. Completion of temperature measurement studies and possible determination of spectral emissivity.

3. Redetermination of vaporization rates of liquid alumina in vacuo for a range of temperatures.

4. Adaptation of quadrupole mass filter to system in event of its arrival.

5. Completion of the determination of the course of crystallization of vapor-deposited $A\ell_2O_3$ from the amorphous to α-$A\ell_2O_3$ states.

(B) MASS-SPECTROMETRIC RESEARCH

The heat of sublimation of BeF_2(s) was obtained from a mass spectrometric study and was presented in NBS Report 8033, pp. 55-59, (July 1, 1963). The reaction of BeF_2(g) with BeO(s) has been studied mass spectrometrically also and is found in NBS Report 8186, pp. 103-112 (Jan. 1, 1964). For the complex specie, Be_2OF_2(g), the enthalpy of reaction and heat of reaction were obtained. In the BeO-$A\ell_2O_3$ system data is being obtained on the 1:1 compound and the 1:3 compound. The only complex vapor specie found above the 1:1 compound is BeOAℓ.

A second Knudsen cell assembly is almost completed for the 60° sector mass spectrometer.

Program Plans

The BeO-$A\ell_2O_3$ system will be concluded by observing the vapor species over the eutectic compositions of these compounds.

Preliminary experiments on the kinetics of vaporization and complex specie formation on the BeF_2-$BeC\ell_2$ are ready to start with the time-of-flight mass spectrometer.

A mass spectrometric study will be attempted with the BeO-H_2O system.

9. EXPERIMENTAL THERMOCHEMISTRY

1. Accomplishments

A redetermination was made of the heat of decomposition of $KC\ell O_4$(c) by a technique slightly modified from that previously employed. The results essentially confirm those published previously by this laboratory.

Using the same technique, we have completed measurements on the decomposition of sodium and potassium chlorates. These results, which will be published in the Journal of Research of NBS, have been used to verify the consistency and reliability of the technique used.

Some data have been obtained on the reaction of hydrazine diperchlorate with chloride solutions. However the reaction has proven to be too slow for satisfactory calorimetry under the present conditions. This study has been temporarily postponed in order to concentrate more intensively on the determination of aluminum borohydride.

Preliminary investigations on $A\ell(BH_4)_3$ were carried out to determine the feasibility of several possible calorimetric reactions. Reactions with N_2 or $C\ell_2$ in a bomb, as well as hydrolysis reactions, were studied. We have decided that chlorination in a flow calorimeter, using standard flame calorimetry techniques, is feasible. A reaction vessel, specially designed for this reaction, has been built and the system calibrated electrically. The analytical methods required to establish the stoichiometry of the calorimetric reactions have been under continued improvement, and we are now able to obtain consistent results although not yet with high precision.

2. Plans for FY 1965

We plan to complete the measurements on $A\ell(BH_4)_3$ during the next quarter. A new sample has been obtained, but detailed analytical data are not yet available. We are also obtaining a highly purified sample of $C\ell_2$ free of oxygen and chlorine oxides for the final determinations.

Upon completion of these measurements we will resume work on the heat of formation of hydrazine diperchlorate, pursuing the solution reaction technique.

10. HIGH-TEMPERATURE MATRIX SPECTROSCOPY

The newly designed electron-bombardment furnace and its associated power supply are virtually complete. They should be ready for matrix spectroscopy within a month. The assembled apparatus will enable infrared observations to be made on matrix deposits of high temperature species over a much greater range than has heretofore been used, especially in the region of low-frequency fundamentals.

PART B. THERMODYNAMIC PROPERTIES OF LIGHT-ELEMENT COMPOUNDS

Chapter B-1

HEAT OF FORMATION OF ALUMINUM CARBIDE

R. C. King and G. T. Armstrong

In an earlier report [1] we described an experimental study in which we measured the heat of combustion of aluminum carbide in oxygen (reaction 1) and derived the heat of formation.

$$A\ell_4C_3(c) + 6O_2(g) = 2A\ell_2O_3(c,\alpha) + 3CO_2(g) \qquad (1)$$

An important and interesting result of the study was the finding that a major fraction of the solid combustion product was delta alumina. The remainder of the product was alpha alumina.

At the time of the earlier report, a major uncertainty in the calculation of the heat of formation of $A\ell_4C_3$ was lack of knowledge of the energy state of the aluminum oxide formed. Recently new information has been presented concerning the energy relationship between delta- and alpha-aluminas, which allows a less ambiguous interpretation of our previous results.

As pointed out earlier the delta alumina was deposited in extremely finely divided form on the wall of the combustion bomb. While on the bomb wall, the oxide appeared white, but once removed from the bomb and placed in a sample container, it appeared to be light gray. Because of this slight discoloration, a qualitative spectrochemical analysis was also performed on samples from two different experiments in order to get information on the purity of the oxide. The same impurities were found in both samples. The results from this analysis are given in Table 1.

Table 1

Qualitative Spectrochemical Analysis of δ-$A\ell_2O_3$ Samples

Element	Percent		Element	Percent
Aℓ	> 10		Mg	0.0001-0.001
Ag	0.0001-0.001		Mn	0.0001-0.001
Au	0.01 -0.1		Ni	0.01 -0.1
B	< 0.0001		Pb	0.0001-0.001
Ca	0.0001-0.001		Pt	0.01 -0.1
Cr	0.01 -0.1		Sn	0.001 -0.01
Cu	0.001 -0.01		Si	0.1 -1.0
Fe	0.01 -0.1		V	0.001 -0.01

The impurities originated from the aluminum carbide sample, and probably also from the platinum foil on the sample container, and from the nichrome fuse and its platinum supports. The indication of a larger amount of silicon in the product than in the $A\ell_4C_3$ is probably the most important change, which can be accounted for either by variability in the sample, or by its being a borderline concentration at about 0.1% in the spectrochemical analyses. No change was made in the calculations as a result of the analysis of the product.

The large fraction of the little-known delta phase in the product raised the question of how much energy difference there is between the delta and alpha crystalline forms of alumina. To obtain this energy difference the energies of combustion observed for aluminum carbide were plotted against the fraction of δ-$A\ell_2O_3$ in the product with the expectation that a linear relation between the two would allow extrapolation to 100% α-$A\ell_2O_3$. The relationship obtained did not allow unambiguous extrapolation. As a result, the value calculated for the energy difference between the two forms of alumina was not very certain and contributed several kcal mole^{-1} to the uncertainty of the value calculated for the heat of formation of the aluminum carbide.

Since these experiments were carried out, additional and more reliable information has become available on the energy difference between the two forms of alumina. Kleppa and Yokokawa [2] have measured the enthalpy difference between δ-$A\ell_2O_3$ and α-$A\ell_2O_3$ by means of solution calorimetry. The samples of delta alumina used in their experiments were obtained in the aluminum carbide combustion experiments described in our previous report [1]. Their experiments on alpha alumina were carried out using samples from several different sources and included one sample prepared by conversion of delta alumina. They found that the heats of solution for the various samples were in agreement. The samples were dissolved in a PbO-BaO-B_2O_3 melt at 705°C. For the conversion of δ-$A\ell_2O_3$ to α-$A\ell_2O_3$ (eq. 2), they obtained the value, $\Delta H^\circ_{298.15} = -2.7 \pm 0.4$ kcal mole^{-1}.

$$\delta\text{-}A\ell_2O_3 \;=\; \alpha\text{-}A\ell_2O_3 \qquad (2)$$

In Table 2 are summarized the observed energies of combustion of aluminum carbide, the fractions of delta phase observed, and the calculated energies of combustion of the aluminum carbide to alpha alumina only. The latter values include a correction for the energy of conversion of δ-$A\ell_2O_3$ to α-$A\ell_2O_3$, based on the work of Kleppa and Yokokawa. The mean value obtained for the energy of combustion of $A\ell_4C_3$ by reaction (1) is: $\Delta E^\circ_{298.15} = -1031.5 \pm 1.1$ kcal mole^{-1}. Conversion to the constant pressure process leads to $\Delta H^\circ_{298.15} = -1033.3$ ± 1.1 kcal mole^{-1}. The uncertainty (1.1 kcal mole^{-1}) is the standard deviation of the mean and includes the uncertainty in the combustion experiments (1.0 kcal mole^{-1}) and the uncertainty (0.4 kcal mole^{-1}) in the energy difference between the aluminas.

Table 2

Heat of Combustion of $A\ell_4C_3$

Expt. No.	$A\ell_2O_3$ $\frac{\delta}{\alpha + \delta}$	$-\Delta U^{\circ}_{298}$ $(A\ell_4C_3)$ (obs)	$-\Delta U^{\circ}_{298}$ $(A\ell_4C_3)$ to α-$A\ell_2O_3$
10	.768	29826.1	29947.6
11	.641	29800.0	29900.6
12	.456	29922.0	29993.6
13	.475	30002.2	30076.8
16	.471	29963.8	30037.7
18	.517	29816.1	29897.2
19	.517	29850.0	29931.1
20	.472	29976.6	30050.7
	Mean	29894.6	29979.4
Standard Deviation of Mean		30.6	25.4
		1028.6 ±1.0 kcal $mole^{-1}$	1031.5 ±.9 kcal $mole^{-1}$

From our data we calculate the heat of formation of $A\ell_4C_3$ to be: $\Delta H f^{\circ}_{298.15}$ $[Al_4C_3(c)] = -49.7 \pm 1.2$ kcal $mole^{-1}$. The following auxiliary data were used in the calculation: $\Delta H f^{\circ}_{298.15}$ $[\alpha\text{-}A\ell_2O_3(s)] = -400.4 \pm 0.3$ kcal $mole^{-1}$ [3]. $\Delta H f^{\circ}_{298.15}$ $[CO_2(g)] = -94.05 \pm 0.01$ kcal $mole^{-1}$ [4]. The uncertainty (1.2 kcal $mole^{-1}$) is the square root of the sum of the squares of the uncertainties assigned to the heat of combustion of the $A\ell_4C_3$, and the heats of formation of the α-$A\ell_2O_3$ and CO_2.

Mah [5] recently measured the heat of combustion of aluminum carbide in oxygen, and calculated the heat of formation to be: $\Delta H f^{\circ}_{298.15} = -53.4 \pm 2.0$ kcal $mole^{-1}$. It is interesting to note that the product alumina in Mah's experiments consisted of very little of a crystalline form of alumina other than α-$A\ell_2O_3$.

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Chapter B-2

REVISED HEATS OF FORMATION OF FLUORIDES

G. T. Armstrong and M. C. Bracken

$A\ell F_3(c)$ $\Delta Hf_{298} = -360 \pm 2$ kcal $mole^{-1}$

Domalski and Armstrong [1] measured the heat of combustion of aluminum in fluorine and found $\Delta H^{o}_{298} = -360.4 \pm 0.3$ kcal $mole^{-1}$. This has involved a recalculation of previously reported data given by Domalski [2].

Gross, Hayman, and Levi [3,4] reported the heat of the reaction, $\frac{3}{2}PbF_2 + A\ell = A\ell F_3 + \frac{3}{2}Pb$, to be -118.53 ± 0.08 kcal $mole^{-1}$. If we modify the heat of formation of PbF_2 given in NBS Circular 500 [5] for a change (-0.84 kcal $mole^{-1}$ [6]) in ΔHf^{o}_{298} [HF (aq)] we obtain -160.2 kcal $mole^{-1}$ for ΔHf^{o}_{298} [PbF_2], and -358.8 kcal $mole^{-1}$ for ΔHf^{o}_{298} [$A\ell F_3$]. Gross, et al. [4] also measured the heat of the reaction $\frac{3}{2}PbF_2 + A\ell + 3NaF = \frac{3}{2}Pb + Na_3A\ell F_3$ and found $\Delta H^{o}_{298} = -138.31 \pm 0.11$ kcal $mole^{-1}$. Combining the results for the two reactions they calculated for the reaction $A\ell F_3 + 3NaF = Na_3A\ell F_3$, $\Delta H^{o}_{298} = -19.78 \pm 0.14$ kcal $mole^{-1}$. This reaction allows calculation of the heat of formation of $A\ell F_3$ independent of the heat of formation of PbF_2. Using Coughlin's data [7] for the heat of formation of NaF, -137.03 kcal $mole^{-1}$, and the heat of formation of cryolite, -788.9 kcal $mole^{-1}$, modified to take into account modified values for ΔHf of $A\ell F_3$ and of HF, we calculate ΔHf^{o}_{298} [$A\ell F_3(c)$] = -358.0 by this method.

Kolesov, Martynov and Skuratov [8] also measured the enthalpy of the reaction between PbF_2 and $A\ell$. They found $\Delta H^{o}_{298} = -117.7 \pm 0.6$ kcal mole. From this value, applying the same data for PbF_2 as before, we calculate ΔHf^{o}_{298} [$A\ell F_3(c)$] = -358.0 kcal $mole^{-1}$. The equilibrium data of Mashovets and Yudin [9] reduced to 298°K using the third law, and then applying the revised heat of formation of HF(g), lead to ΔHf [$A\ell F_3(c)$] = -357.7 kcal $mole^{-1}$.

In selecting 360 kcal $mole^{-1}$ as the best value we give greater weight to the direct combustion determination, but assign a relatively large uncertainty to take account of possible systematic errors in that value and also to give weight to the determinations by other reaction processes.

$BeF_2(c)$ $\Delta Hf^{o}_{298} = -243 \pm 3$ kcal mole^{-1}

The heats of reaction of BeO and of BeF_2 with aqueous HF were determined by Kolesov, Popov and Skuratov [10], who found -24.17 ±0.12 and -8.04 ±0.08 kcal mole^{-1} respectively for the standard heats of reaction at 298°C. Applying to these data revised values for the heat of formation of HF(aq) [6], we calculate (see Churney [2]) ΔH^{o}_{f298} [$BeF_2(c)$] = -242.27 kcal mole^{-1}.

Recent work still in progress by Gross on the reaction of Be with PbF_2 [12] gives heats which are somewhat sensitive to the ratio of PbF_2 to Be. The heat, however, appears to become constant at -83.8 kcal mole at the higher ratios. This value combined with ΔH^{o}_{f298} [$PbF_2(c)$] = -160.2 kcal mole^{-1} [see $A\ell F_3(c)$] gives ΔH^{o}_{f298} [$BeF_2(s)$] = -244.0 kcal mole^{-1}. The degree of crystallinity of the BeF_2 is not constant in these experiments, and the results are subject to a correction for the difference between the glassy and the crystalline forms. A recent study by Taylor [13] indicates this difference to be 1.1 kcal mole^{-1}, with the crystalline form being the more stable.

Direct combustion of beryllium in fluorine has not yet led to published conclusions [14] but the heat measurements that have been made are consistent with the measurements described above. The results of Kolesov, et al. are dependent on the heat of formation of BeO, in which the uncertainty may be as great as 3 kcal mole^{-1}.

An intermediate value of -243 kcal mole^{-1} is selected as the best value.

MgF_2 $\Delta Hf^{o}_{298} = -265 \pm 2$ kcal mole^{-1}

Rudzitis and Hubbard [15] have informally reported the heat of combustion of magnesium in fluorine to be -264.9 kcal mole^{-1}.

Domange [16] studied the equilibrium constant of the reaction, $MgF_2(c) + H_2O(g) = MgO(c) + 2HF(g)$. A third law treatment of their data leads to a value of $\Delta H^{o}_{298} = 45.94$ kcal mole^{-1} for this reaction. Applying the values -64.8 [6], -143.7 [17], and -57.80 [5] kcal mole^{-1} respectively for ΔH^{o}_{f298} of HF, MgO, and H_2O, we obtain for $MgF_2(c)$ ΔH^{o}_{f298} = -261.4 kcal mole^{-1}.

Von Wartenberg [18] determined the heat of solution of magnesium in aqueous hydrofluoric acid ($HF \cdot 80\ H_2O$) and found $\Delta H = -109.5 \pm 0.7$ kcal mole^{-1}. Using ΔH^{o}_{f298} ($HF \cdot 80\ H_2O$) = -76.33 kcal mole^{-1} [6], we calculate ΔH^{o}_{f298} [$MgF_2(c)$] = -262.2 kcal mole^{-1}.

Torgeson and Sahama [19] determined the heat of reaction of $Mg(OH)_2$ with aqueous hydrofluoric acid (20.1% HF by weight) at 73.7°C to be -29.090 kcal $mole^{-1}$, and the enthalpy difference of the resulting aqueous solution at 25°C and 73.7°C to be -1.620 kcal $mole^{-1}$ of $Mg(OH)_2$. They also measured the heat of hydration of MgO, and found it to be -8.85 kcal $mole^{-1}$. Using these data, the specific heat of aqueous HF from Thorvaldson and Bailey [20], the enthalpy of MgF_2 from Furukawa et al. [21], and ΔHf^{o}_{298} [$HF \cdot 4.415\ H_2O$] = -76.12 kcal $mole^{-1}$ [6], we calculate ΔHf^{o}_{298} [$MgF_2(c)$] = -267.4 kcal $mole^{-1}$.

Gross, Hayman, and Levi [3] measured the heat of the reaction, $Mg(c) + PbF_2(c) = MgF_2(c) + Pb(c)$, and after correcting for the formation of a Mg-Pb alloy in some experiments calculated $\Delta H^{o}_{298} = -109.5 \pm 1.5$ kcal $mole^{-1}$. Using ΔHf^{o}_{298} [$PbF_2(c)$] = -160.2 kcal $mole^{-1}$ [see $A\ell F_3(c)$], we calculate ΔHf^{o}_{298} [$MgF_2(c)$] = -269.7 kcal $mole^{-1}$.

The mean of the indirect methods for determining the heat of formation of $MgF_2(c)$ is -265.2 kcal $mole^{-1}$, which is in good agreement with the value found by the direct combustion of the metal in fluorine. A value of -265 ±2 kcal $mole^{-1}$ is selected as the best value.

LiF(c) $\Delta Hf^{o}_{298} = -147.1 \pm 0.5$ kcal $mole^{-1}$

Stephenson, Hopkins, and Wulff [22] determined the heat of solution of LiF to be $\Delta H^{o}_{298} = 1.070 \pm 0.050$ kcal $mole^{-1}$. Combining this value with ΔHf^{o}_{298} [$Li^{+}(aq)$] = -66.55 kcal $mole^{-1}$ [5], and ΔHf^{o}_{298} [$F^{-}(aq)$] = -79.50 kcal $mole^{-1}$ [6], these data are combined to give ΔHf^{o}_{298} [$LiF(c)$] = -147.1 kcal $mole^{-1}$. The uncertainty assigned above is principally due to the uncertainty in the heat of formation of the aqueous fluoride ion.

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Chapter B-3

CALCULATION OF THE EQUILIBRIUM COMPOSITION, ENTHALPY, ENTROPY, AND DENSITY OF THE AIR-ALUMINUM GAS MIXTURE GENERATED IN AN EXPLODING WIRE EXPERIMENT

by

Klaus K. Neumann and Esther C. Cassidy

1. INTRODUCTION

In the past few years numerous papers have been written on exploding wire phenomena [1, 2], and many varied applications of its electrical discharge method have been devised. This paper presents a theoretical calculation of the composition, entropy, enthalpy and density, as functions of pressure and temperature, of the gas mixture produced by the explosion of an aluminum wire in an air environment. The mixture, though it is generated by a transient method, is assumed to pass through a series of high-temperature, high-pressure states in which all of the particles in the mixture are in thermodynamic equilibrium. The assumption of thermodynamic equilibrium is reasonable, inasmuch as the time (10^{-5} to 10^{-12} sec)[3] required for establishment of equilibrium conditions is very short compared to the time required for the explosion. Preliminary experiments by the authors have shown that the current in the discharge lasts about 10^{-4} sec, and that the radiation emitted lasts about 4×10^{-3} sec.

The calculations were made for six constant pressures between 0.01 and 1000 atm, at each 500° temperature interval between 1500 and 6000° K. The computations were made at constant pressures, rather than at constant densities, so that the results could be compared more readily with experimental results, the measurement of pressure in exploding wire experiments being more feasible than the measurement of density.

2. THE EXPLOSION MIXTURE

The mixture considered was that generated by the explosion of an aluminum wire in a closed vessel containing air under normal laboratory conditions. The system before explosion was assumed to be 100 parts air and 10 parts Al_2 (79 parts N_2, 21 parts O_2 and 10 parts Al_2). These ratios were determined primarily by the conditions of experiments now being performed by the authors in an effort to develop a suitable system and suitable methods for direct measurement of thermodynamic data under the transient high-temperature, high-pressure conditions of the explosion.

The components of the explosion mixture were assumed to be $Al_2, N_2, O_2, Al, AlO, Al_2O, Al_2O_2, N, NO, NO_2, N_2O$ and O, all in the gas phase only. The solid and liquid phases were not considered, inasmuch as the reaction rates to condensed liquid and/or solid particles are much slower than the reaction rates between gaseous particles. Other possible components, such as N_2O_4, the ions O_2^+, N_2^+, etc, were neglected inasmuch as they make up only a very small percentage of the mixture. Still other components, such as the aluminum-nitrides, were omitted because of the lack of data in the literature.

Free electrons and the ion Al^+ were also not included. This latter assumption is in error at the higher temperatures (near 6000° K) and lower pressures (near 0.01 atm), because some of the aluminum atoms are surely ionized in this region. However, one may consider that the Al^+ concentrations are included in the calculated neutral Al concentrations. The calculated enthalpies in this region will also be slightly lower than they should be, inasmuch as the ionization energies of the Al are not included. In the other pressure–temperature regions of the calculation, the error due to the omission of ions and free electrons is small, because at higher pressures the aluminum oxides are the predominant aluminum component. Therefore, the number of Al^+ ions would be very small, since there are only a few Al atoms from which the Al^+ ions may be formed.

One further assumption, which may introduce error in the calculations, was as follows. The molecule $Al_2O_3(g)$ was not included because of the lack of input data. To the authors knowledge, no observations of or data on gaseous Al_2O_3 have been published. The only reference uncovered was that of Medvedev [4] who, although he has not observed Al_2O_3 (g), states that he believes it may be present in the experimental mixtures of Brewer and Searcy [5].

3. THE INPUT DATA

In order to ensure consistency, all of the input data were taken from McBride et al [6]. Some of the data in this reference are calculated values, rather than experimentally observed values. However, the authors have noted that observed data for AlO, Al_2O, Al_2O_2 and Al_2 [7,8,9], are in fairly good agreement with those of McBride et al. In any case, one may say, as a limit for the errors, that the relative error in each computed volume fraction must be smaller than the sum of the relative errors in the input equilibrium constants [13].

4. METHOD OF CALCULATION

The method of calculation is similar to that described by Neumann and Knoche [10]. The computations were performed with the aid of a high-speed digital computer, using the general-purpose machine program OMNITAB [11].

The enthalpy $H_{j,T}$ and entropy $S_{j,p_o,T}$ of each component j (where j = 1 to 12), at the normal pressure p_o = 1 atm for each 500° temperature interval between 1500 and 6000°K, were taken as the input data. The entropy $S_{j,p,T}$ at p = 0.01, 0.1, 1, 10, 100 and 1000 atm for each component j and each temperature T (500° intervals between 1500 and 6000°K) was calculated from the following equation:

$$S_{j,p,T} = S_{j,p_o,T} - R \ln p \qquad (1)$$

where R is the universal gas constant = 1.98726 cal/mole °K.

The equilibrium constant $K_{j,p,T}$ for each component at each pressure and each temperature was calculated from

$$R \ln K_{j,p,T} = \left(S_{j,p,T} - \frac{H_{j,T}}{T}\right) - \sum_{j'=1}^{j=3} v_{j',j} \left(S_{j',p,T} - \frac{H_{j',p}}{T}\right). \tag{2}$$

At this point, for the sake of simplicity, the indices p and T, which define the pressure and temperature levels for each parameter, will be dropped from the equations. It is to be understood that the method described refers to the calculations at any one given pressure and temperature. The index j' refers to the prime components of the mixture. For the method of calculation used here, these prime components must contain at least one atom of each of the chemical elements (aluminum, nitrogen, and oxygen) contained in the mixture. In this paper, the molecules Al_2, N_2, and O_2 (with the index $j' = 1, 2, 3$) were taken as the prime components. $v_{j,j'}$ is an array of "reaction numbers", consisting of three columns ($j' = 1$ to 3) and 12 rows ($j = 1$ to 12), which are taken from the coefficients in the chemical reaction equations for each molecule. For this purpose, the equations for the reaction must be written in a form which contains only prime components and one other component. Therefore, every $v_{j',j}$ value gives the number of moles of the prime components j' which the reaction consumes to form one mole of the product component j.

The calculation of the composition of the gas-mixture, as a function of pressure and temperature, begins as follows.

Assuming an ideal behavior of the gas, the volume-fraction r_j of each component is computed from the mass-balance equations (3) and from the equilibrium equations (4):

$$\sum_{j=1}^{12} h_{k,j} \, r_j = b_k \tag{3}$$

and

$$r_j = K_j \prod_{j'=1}^{3} r_{j'}^{\,v_{j',j}} \quad . \tag{4}$$

For this problem there are three mass-balance equations (always equal in number to the number of prime components) and nine equilibrium equations (one for each of the other components). The index k refers to the mass-balance equations. For $k = 1$, the coefficients $h_{1,j}$ of the volume fractions are always equal to 1, and equation (3) simply states that the sum of all the volume fractions is equal to $b_1 = 1$:

$$\sum_{j=1}^{12} r_j = 1. \tag{5}$$

For $k = 2$ and $h_{2,j}$ equal to the ratio between O and N in the mixture:

$$\begin{aligned} b_k = {} & 0r_1 - 42r_2 + 158r_3 + 0r_4 + 79r_5 \\ & + 79r_6 + 158r_7 - 21r_8 + 58r_9 \\ & + 137r_{10} + 37r_{11} + 79r_{12} = 0. \end{aligned} \tag{6}$$

This equation was reduced from

$$\frac{0r_1+0r_2+2r_3+0r_4+1r_5+1r_6+2r_7+0r_8+1r_9+2r_{10}+1r_{11}+1r_{12}}{0r_1+2r_2+0r_3+0r_4+0r_5+0r_6+0r_7+1r_8+1r_9+1r_{10}+2r_{11}+0r_{12}} = \frac{21}{79} \; . \tag{7}$$

The coefficients here are simply the number of parts of O and N in each component of the mixture. A similar equation for the ratio between all the Al components and all the N components in the mixture reduces to the following equation for $k = 3$:

$$\begin{aligned} b_k = {} & 158r_1 - 20r_2 + 0r_3 + 79r_4 + 79r_5 + 158r_6 \\ & + 158r_7 - 10r_8 - 10r_9 - 10r_{10} - 20r_{11} \\ & + 0r_{12} = 0 \ . \end{aligned} \tag{8}$$

From equations (5), (6), and (8) one sees that b_1 is equal to 1 and that b_2 and b_3 must be equal to zero.

In order to simplify the calculations, equations (3) and (4) were written in logarithmic form:

$$\sum_{j=1}^{12} h_{k,j} \bullet^{\ln r_j} = b_k \tag{9}$$

and

$$\ln r_j = \ln K_j + \sum_{j'=1}^{3} v_{j',j} \ln r_{j'} . \tag{10}$$

We now have a system of 12 equations, three from equation (9) and nine from equation (10), with 12 unknown r_j .

To begin the calculations, three approximate values are estimated for $r_{j'}$, and the other r_j are computed from equation (10). These computed approximate values for r_j will not satisfy the three transcendental equations (9). However, a systematic iteration may be performed with the aid of the equation (9) written in the following form:

$$b_k - \sum_{j=1}^{12} h_{k,j} e^{\ln r_j} = b_k - \sum_{j=1}^{12} h_{k,j} r_j = \Delta b_k . \tag{11}$$

For convenience, equation (11) may be reduced to:

$$F_k (r_1, r_2, r_3) = \Delta b_k \tag{12}$$

where F_k is simply the function $[b_k - \sum_{j=1}^{12} h_{k,j} r_j]$

written in a form which indicates its dependence on the three $r_{j'}$. Δb_k in equation (12) will remain unequal to zero as long as r_1, r_2, and r_3 are not properly determined. When $\Delta b_k = 0$, the computation of the r_j is complete, and the zero points of the three functions F_k are determined.

For this paper, a generalized Newtonian method [12] was used to approach the zero points of F_k (where $\Delta b_k = 0$). Each function was approximated by its tangent as follows:

$$\Delta F_k = \left(\frac{\partial F_k}{\partial \ln r_2}\right) \cdot \Delta \ln r_1 + \left(\frac{\partial F_k}{\ln r_2}\right) \cdot \Delta \ln r_2 + \left(\frac{\partial F_k}{\partial \ln r_3}\right) \cdot \Delta \ln r_3 \qquad (13)$$

Zero values for F_k are then approximated by substituting F_k (i.e. Δb_k) for ΔF_k in equation (13). Then, from equations (12) and (13), one may write:

$$\Delta b_k = \sum_{j'=1}^{3} \frac{\partial F_k}{\partial \ln r_{j'}} \Delta \ln r_{j'} . \qquad (14)$$

Further, from equations (11) and (12):

$$\left(\frac{\partial F_k}{\partial \ln r_{j'}}\right) = \sum_{j=1}^{12} h_{k,j}\left(\frac{\partial e^{\ln r_j}}{\partial \ln r_{j'}}\right) = \sum_{j=1}^{12} h_{k,j} \frac{\partial e^{\ln r_j}}{\partial \ln r_j} \frac{\partial \ln r_j}{\partial \ln r_{j'}} = \ln e \sum_{j=1}^{12} h_{k,j}\left(\frac{\partial \ln r_j}{\partial \ln r_{j'}}\right) e^{\ln r_j}$$

$$= \sum_{j=1}^{12} h_{k,}\left(\frac{\partial \ln r_j}{\partial \ln r_{j'}}\right) \cdot r_j , \qquad (15)$$

and from equation (10):

$$\left(\frac{\partial \ln r_j}{\partial \ln r_{j'}}\right) = v_{j',j} \quad . \tag{16}$$

Therefore,

$$\left(\frac{\partial F_k}{\partial \ln r_{j'}}\right) = \sum_{j=1}^{12} h_{k,j} \ v_{j',j} \ r_j = g_{j',k} \tag{17}$$

where $g_{j',k} = \left(\frac{\partial F_k}{\partial \ln r_{j'}}\right)$. The three equations(14) may then be written simply as :

$$\Delta b_k = \sum_{j'=1}^{3} g_{j',k} \ . \ \Delta \ln r_{j'} \ . \tag{18}$$

In summary, the three correct $r_{j'}$ (the volume-fractions of the prime components Al_2, N_2 and O_2) are computed by an iterative method from the set of three linear equations (18). The array $g_{j',k}$ are given by equation (17), and the three Δb_k are given by equation (11). The calculations are begun by substituting approximate values for $r_{j'}$ in equation (18). The computed value for $\Delta \ln r_{j'}$ is then added to the old r_j as follows:

$$\ln r_{j'\,new} = \ln r_{j'\,old} + \Delta \ln r_{j'} \ . \tag{19}$$

Ln $r_{j'new}$ is then substituted in equation (18), and the iteration is continued until $\Delta \ln r_{j'} = 0$. At this point, the other r_j (the volume fractions of the other nine components) have also been properly determined from equation (10), and the calculation of the composition of the gas-mixture, i.e. of the volume-fraction r_j of each component is complete. This calculation is performed for each desired pressure and temperature interval.

In a second set of calculations, the enthalpy per unit mass H, the entropy per unit mass S, and the density D of the mixture at each desired pressure and temperature were calculated from the following equations:

$$H = \frac{\sum_{j=1}^{12} r_j H_j}{\sum_{j=1}^{12} r_j M_j} \tag{20}$$

$$S = \frac{\sum_{j=1}^{12} r_j (S_j - R \ln r_j)}{\sum_{j=1}^{12} r_j M_j} \tag{21}$$

and

$$D = \frac{p}{RT} \sum_{j=1}^{12} r_j M_j \ . \tag{22}$$

The computed values (from the first set of calculations) for the volume-fractions r_j, the molar enthalpies H_j, the molar entropies S_j, and the molecular weights M_j were used as input data. For consistency, the reference elements and the base for the enthalpies assigned by McBride et al [6]. ($Al_{crystal}$, $N_{2\,gas}$ and $O_{2\,gas}$ and a zero value of 298.15°K) were also used for these calculations.

5. RESULTS AND DISCUSSION

The results of the calculations, i.e., the concentrations of the various components in the explosion mixture and the enthalpy, entropy and density of the mixture at the various pressures and temperatures, are presented in Tables 1 thru 6. The concentrations of the various components are also presented graphically in figures 1 through 6. The graphical presentation is of interest, inasmuch as it provides an overall picture of the composition and state of the explosion mixture at the various levels of pressure and temperature. Further, it may serve as a guide to the conditions which are more favorable for experimental observation of various components in the mixture. Some of the points of interest which may be noted from the figures for this mixture are discussed in the following paragraphs:

1.) The concentration of Al_2 molecules is very small (always less than 0.01% of the mixture) for all the levels of pressure and temperature considered. One may, therefore, conclude that for observations of the Al_2 molecule the wire should not be exploded in an air or oxygen environment, where the calculations indicate that the formation of oxides will predominate the mixture. A noble gas environment should rather be preferred for Al_2 observations.

2.) At the lower temperatures (less than 3500°K) nearly all the aluminum in the mixture is in the form Al_2O_2 for all pressure levels. This system should, therefore, be favorable for observation of the Al_2O_2 molecule.

3.) At the lower pressures the aluminum oxides are the predominent aluminum components up to 3500° K. Beyond 3500° K, the oxide concentrations drop to zero, and the Al concentration increases. Therefore, as a rough estimate, if spectroscopic observations of the explosion show oxide bands and if it has been determined that the mixture passes through a series of instantaneous equilibrium states, one may conclude that the temperature of the explosion mixture does not exceed 3500° K. In making such an estimate, however, one must be sure that the observed oxide bands are due to radiation from an equilibrium state rather than from chemical luminescence.

4.) At the lower pressures, the figures show that the concentration of a given oxide is high only in a very small temperature range (e.g. the Al_2O concentration is high only between 2000 and 3000 °K). At the higher pressures, the temperature range for high concentration of a given oxide is larger (e.g. Al_2O concentration is high between 3000 and 6000 °K).

The entropies, enthalpies, and densities of the explosion mixture are shown graphically in figures 7 through 9. Figure 10 is a Mollier Diagram showing the entropy of the mixture at the various pressures and temperatures plotted as a function of the enthalpy. This latter diagram is of particular interest as a guide in the practical planning of experiments. To use the diagram effectively, one must assume the changes from one equilibrium state to another, in the various stages of the explosion, to be adiabatic. Further, although parts of the explosion are surely not reversible, one may, in order to approach suitable conditions for experiment, assume that these changes are isentropic. Under these assumptions, one may follow an isentrope on the diagram (e.g. the isentrope 2.0 cal/g °K) from pressure to pressure, and determine from the intersecting isotherms what the corresponding temperature change would be (e.g. from approximately 6000°K at 1000 atm to approximately 2500 °k at 1 atm). Further, the approximate energy dissipated in the process may be determined from the enthalpy scale (e.g. for the above case about 1700 cal/g).

In conclusion, it is hoped that the method of calculation, which has been described in detail in the preceding pages, will be of assistance in future thermodynamic calculations, and further that such calculations will in turn serve as a guide to favorable conditions for future exploding wire experiments.

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Table 1. Equilibrium Composition, Entropy, Enthalpy, and Density of the Air-Aluminum Gas Mixture Generated in an Exploding Wire Experiment.

PRESSURE = 0.01 ATM.

TEMPERATURE	1500	2000	2500	3000	3500
AL2	8.374E-21	2.652E-13	1.355E-09	8.832E-08	7.748E-08
N2	7.894E-01	7.744E-01	7.194E-01	6.082E-01	5.611E-01
O2	1.096E-01	1.173E-01	1.039E-01	2.810E-02	2.789E-03
AL	1.055E-09	3.061E-05	5.891E-03	9.229E-02	1.390E-01
AL O	1.213E-05	2.966E-03	2.963E-02	3.466E-02	4.082E-03
AL2 O	2.381E-04	2.650E-02	6.626E-02	1.440E-02	1.072E-04
AL2 O2	9.974E-02	7.041E-02	8.057E-03	1.238E-04	7.070E-08
N	5.706E-13	8.455E-09	2.652E-06	1.166E-04	1.786E-03
N O	9.488E-04	5.979E-03	1.612E-02	1.589E-02	8.037E-03
N O2	3.258E-07	6.850E-07	8.929E-07	2.957E-07	3.467E-08
N2 O	4.990E-09	2.910E-08	7.556E-08	7.043E-08	3.569E-08
O	1.453E-05	2.484E-03	5.072E-02	2.062E-01	2.831E-01

TEMPERATURE	4000	4500	5000	5500	6000
AL2	3.894E-08	2.120E-08	1.153E-08	5.982E-09	3.476E-09
N2	5.488E-01	5.060E-01	3.863E-01	1.972E-01	6.165E-02
O2	3.240E-04	5.563E-05	1.196E-05	2.895E-06	8.897E-07
AL	1.407E-01	1.370E-01	1.261E-01	1.089E-01	9.653E-02
AL O	4.928E-04	8.744E-05	1.927E-05	4.753E-06	1.482E-06
AL2 O	1.211E-06	3.269E-08	1.497E-09	9.403E-11	9.353E-12
AL2 O2	9.525E-11	4.743E-13	5.294E-15	9.706E-17	3.474E-18
N	1.417E-02	6.912E-02	2.227E-01	4.653E-01	6.391E-01
N O	3.972E-03	2.122E-03	1.086E-03	4.610E-04	1.669E-04
N O2	4.654E-09	8.656E-10	1.789E-10	3.344E-11	6.123E-12
N2 O	1.831E-08	9.896E-09	4.714E-09	1.495E-09	3.196E-10
O	2.915E-01	2.856E-01	2.637E-01	2.282E-01	2.025E-01

TEMP.	H	S	D
1500.	2.940E 01	2.113E 00	2.782E-06
2000.	2.305E 02	2.226E 00	2.053E-06
2500.	6.334E 02	2.404E 00	1.537E-06
3000.	1.493E 03	2.714E 00	1.085E-06
3500.	2.046E 03	2.888E 00	8.544E-07
4000.	2.292E 03	2.953E 00	7.369E-07
4500.	2.722E 03	3.054E 00	6.359E-07
5000.	3.738E 03	3.267E 00	5.264E-07
5500.	5.618E 03	3.624E 00	4.131E-07
6000.	7.410E 03	3.937E 00	3.357E-07

Table 2. Equilibrium Composition, Entropy, Enthalpy, and Density of the Air-Aluminum Gas Mixture Generated in an Exploding Wire Experiment.

PRESSURE = 0.1 ATM.

TEMPERATURE	1500	2000	2500	3000	3500
AL2	8.388E-22	3.492E-14	3.709E-10	6.214E-08	5.128E-07
N2	7.895E-01	7.821E-01	7.430E-01	6.790E-01	5.868E-01
O2	1.096E-01	1.114E-01	1.185E-01	6.940E-02	1.810E-02
AL	1.055E-10	3.511E-06	9.742E-04	2.447E-02	1.130E-01
AL O	3.838E-06	1.049E-03	1.655E-02	4.569E-02	2.676E-02
AL2 O	7.541E-05	1.075E-02	6.124E-02	5.039E-02	5.718E-03
AL2 O2	9.992E-02	8.809E-02	2.515E-02	2.153E-03	3.040E-05
N	1.804E-13	2.686E-09	8.520E-07	3.894E-05	5.773E-04
N O	9.485E-04	5.856E-03	1.749E-02	2.638E-02	2.094E-02
N O2	1.030E-06	2.068E-06	3.272E-06	2.441E-06	7.281E-07
N2 O	1.578E-08	9.061E-08	2.636E-07	3.910E-07	3.008E-07
O	4.592E-06	7.653E-04	1.712E-02	1.025E-01	2.280E-01

TEMPERATURE	4000	4500	5000	5500	6000
AL2	3.780E-07	2.216E-07	1.348E-07	8.166E-08	4.794E-08
N2	5.585E-01	5.419E-01	4.972E-01	3.970E-01	2.455E-01
O2	2.961E-03	5.620E-04	1.368E-04	3.897E-05	1.216E-05
AL	1.386E-01	1.400E-01	1.363E-01	1.272E-01	1.133E-01
AL O	4.642E-03	8.986E-04	2.229E-04	6.444E-05	2.035E-05
AL2 O	1.124E-04	3.436E-06	1.873E-07	1.490E-08	1.509E-09
AL2 O2	8.458E-08	5.013E-10	7.088E-12	1.785E-13	6.556E-15
N	4.520E-03	2.261E-02	7.989E-02	2.087E-01	4.032E-01
N O	1.211E-02	6.981E-03	4.166E-03	2.400E-03	1.231E-03
N O2	1.357E-07	2.863E-08	7.347E-09	2.020E-09	5.285E-10
N2 O	1.782E-07	1.066E-07	6.494E-08	3.494E-08	1.489E-08
O	2.785E-01	2.870E-01	2.820E-01	2.646E-01	2.367E-01

TEMP.	H	S	D
1500.	2.907E 01	1.979E 00	2.782E-05
2000.	1.949E 02	2.073E 00	2.074E-05
2500.	5.059E 02	2.211E 00	1.589E-05
3000.	9.885E 02	2.385E 00	1.219E-05
3500.	1.790E 03	2.632E 00	9.021E-06
4000.	2.197E 03	2.742E 00	7.486E-06
4500.	2.474E 03	2.807E 00	6.536E-06
5000.	2.925E 03	2.901E 00	5.698E-06
5500.	3.807E 03	3.069E 00	4.828E-06
6000.	5.292E 03	3.326E 00	3.942E-06

Table 3. Equilibrium Composition, Entropy, Enthalpy, and Density of the Air-Aluminum Gas Mixture Generated in an Exploding Wire Experiment.

PRESSURE = 1 ATM.

TEMPERATURE	1500	2000	2500	3000	3500
AL2	8.388E-23	3.893E-15	7.904E-11	2.079E-08	6.422E-07
N2	7.895E-01	7.854E-01	7.599E-01	7.168E-01	6.553E-01
O2	1.095E-01	1.086E-01	1.161E-01	1.006E-01	5.278E-02
AL	1.055E-11	3.707E-07	1.422E-04	4.474E-03	3.999E-02
AL O	1.213E-06	3.458E-04	7.563E-03	3.182E-02	5.113E-02
AL2 O	2.385E-05	3.746E-03	4.088E-02	6.421E-02	3.868E-02
AL2 O2	9.997E-02	9.586E-02	5.257E-02	1.045E-02	1.111E-03
N	5.703E-14	8.508E-10	2.724E-07	1.265E-05	1.928E-04
N O	9.484E-04	5.795E-03	1.751E-02	3.263E-02	3.778E-02
N O2	3.258E-06	6.394E-06	1.026E-05	1.150E-05	7.096E-06
N2 O	4.992E-08	2.842E-07	8.441E-07	1.572E-06	1.814E-06
O	1.451E-06	2.389E-04	5.356E-03	3.899E-02	1.231E-01

TEMPERATURE	4000	4500	5000	5500	6000
AL2	2.450E-06	2.093E-06	1.406E-06	9.438E-07	6.325E-07
N2	5.854E-01	5.576E-01	5.388E-01	5.011E-01	4.280E-01
O2	1.812E-02	4.804E-03	1.336E-03	4.302E-04	1.553E-04
AL	1.116E-01	1.360E-01	1.392E-01	1.367E-01	1.301E-01
AL O	2.924E-02	8.073E-03	2.249E-03	7.279E-04	2.641E-04
AL2 O	5.700E-03	3.001E-04	1.931E-05	1.810E-06	2.250E-07
AL2 O2	3.357E-05	4.049E-07	7.224E-09	2.279E-10	1.105E-11
N	1.463E-03	7.251E-03	2.629E-02	7.411E-02	1.683E-01
N O	3.068E-02	2.070E-02	1.355E-02	8.958E-03	5.810E-03
N O2	2.690E-06	7.853E-07	2.362E-07	7.928E-08	2.818E-08
N2 O	1.462E-06	1.014E-06	6.956E-07	4.635E-07	2.934E-07
O	2.178E-01	2.652E-01	2.786E-01	2.780E-01	2.674E-01

TEMP.	H	S	D
1500.	2.897E 01	1.845E 00	2.782E-04
2000.	1.801E 02	1.932E 00	2.082E-04
2500.	4.223E 02	2.038E 00	1.624E-04
3000.	7.587E 02	2.161E 00	1.291E-04
3500.	1.255E 03	2.313E 00	1.018E-04
4000.	1.917E 03	2.490E 00	7.944E-05
4500.	2.318E 03	2.585E 00	6.711E-05
5000.	2.620E 03	2.649E 00	5.904E-05
5500.	3.035E 03	2.727E 00	5.213E-05
6000.	3.717E 03	2.846E 00	4.535E-05

Table 4. Equilibrium Composition, Entropy, Enthalpy, and Density of the Air-Aluminum Gas Mixture Generated in an Exploding Wire Experiment.

PRESSURE = 10 ATM.

TEMPERATURE	1500	2000	2500	3000	3500
AL2	8.384E-24	4.042E-16	1.241E-11	5.518E-09	2.495E-07
N2	7.895E-01	7.866E-01	7.719E-01	7.380E-01	6.994E-01
O2	1.095E-01	1.076E-01	1.091E-01	1.099E-01	8.542E-02
AL	1.054E-12	3.775E-08	1.781E-05	7.286E-04	7.879E-03
AL O	3.836E-07	1.109E-04	2.905E-03	1.714E-02	4.055E-02
AL2 O	7.542E-06	1.224E-03	1.969E-02	5.636E-02	6.048E-02
AL2 O2	9.999E-02	9.865E-02	7.764E-02	3.032E-02	6.990E-03
N	1.803E-14	2.692E-10	8.677E-08	4.056E-06	6.298E-05
N O	9.484E-04	5.772E-03	1.711E-02	3.461E-02	4.966E-02
N O2	1.031E-05	2.005E-05	3.074E-05	4.034E-05	3.753E-05
N2 O	1.579E-07	8.963E-07	2.630E-06	5.352E-06	7.794E-06
O	4.588E-07	7.516E-05	1.641E-03	1.288E-02	4.949E-02

TEMPERATURE	4000	4500	5000	5500	6000
AL2	3.096E-06	1.044E-05	1.187E-05	9.418E-06	7.009E-06
N2	6.503E-01	5.954E-01	5.622E-01	5.413E-01	5.129E-01
O2	4.939E-02	2.342E-02	9.584E-03	3.755E-03	1.555E-03
AL	3.964E-02	9.605E-02	1.278E-01	1.365E-01	1.369E-01
AL O	5.426E-02	3.982E-02	1.750E-02	6.794E-03	2.782E-03
AL2 O	3.762E-02	1.046E-02	1.382E-03	1.688E-04	2.496E-05
AL2 O2	1.157E-03	9.858E-05	4.379E-06	1.987E-07	1.227E-08
N	4.874E-04	2.368E-03	8.488E-03	2.435E-02	5.823E-02
N O	5.338E-02	4.724E-02	3.708E-02	2.751E-02	2.012E-02
N O2	2.445E-05	1.252E-05	5.476E-06	2.275E-06	9.771E-07
N2 O	8.482E-06	7.565E-06	6.151E-06	4.680E-06	3.520E-06
O	1.137E-01	1.851E-01	2.359E-01	2.596E-01	2.675E-01

TEMP.	H	S	D
1500.	2.894E 01	1.711E 00	2.783E-03
2000.	1.748E 02	1.795E 00	2.085E-03
2500.	3.666E 02	1.880E 00	1.649E-03
3000.	6.438E 02	1.981E 00	1.330E-03
3500.	9.649E 02	2.080E 00	1.093E-03
4000.	1.395E 03	2.194E 00	8.946E-04
4500.	1.937E 03	2.322E 00	7.281E-04
5000.	2.370E 03	2.413E 00	6.182E-04
5500.	2.702E 03	2.477E 00	5.449E-04
6000.	3.069E 03	2.540E 00	4.861E-04

Table 5. Equilibrium Composition, Entropy, Enthalpy, and Density of the Air-Aluminum Gas Mixture Generated in an Exploding Wire Experiment.

PRESSURE = 100 ATM.

TEMPERATURE	1500	2000	2500	3000	3500
AL2	8.381E-25	4.091E-17	1.527E-12	1.109E-09	7.177E-08
N2	7.895E-01	7.869E-01	7.780E-01	7.543E-01	7.224E-01
O2	1.095E-01	1.072E-01	1.045E-01	1.058E-01	9.894E-02
AL	1.053E-13	3.796E-09	1.975E-06	1.033E-04	1.336E-03
AL O	1.213E-07	3.522E-05	9.973E-04	7.536E-03	2.340E-02
AL2 O	2.385E-06	3.913E-04	7.498E-03	3.515E-02	5.923E-02
AL2 O2	10.000E-02	9.957E-02	9.156E-02	5.869E-02	2.330E-02
N	5.698E-15	8.510E-11	2.754E-08	1.296E-06	2.023E-05
N O	9.483E-04	5.763E-03	1.681E-02	3.433E-02	5.432E-02
N O2	3.260E-05	6.323E-05	9.350E-05	1.241E-04	1.398E-04
N2 O	4.995E-07	2.832E-06	8.206E-06	1.697E-05	2.741E-05
O	1.450E-07	2.372E-05	5.078E-04	3.995E-03	1.684E-02

TEMPERATURE	4000	4500	5000	5500	6000
AL2	1.231E-06	9.242E-06	3.278E-05	5.551E-05	5.850E-05
N2	6.910E-01	6.560E-01	6.155E-01	5.791E-01	5.528E-01
O2	7.750E-02	5.201E-02	3.193E-02	1.857E-02	1.023E-02
AL	7.900E-03	2.856E-02	6.714E-02	1.047E-01	1.250E-01
AL O	4.285E-02	5.582E-02	5.309E-02	3.668E-02	2.061E-02
AL2 O	5.926E-02	4.364E-02	2.203E-02	7.001E-03	1.690E-03
AL2 O2	7.222E-03	1.939E-03	4.032E-04	5.797E-05	6.740E-06
N	1.588E-04	7.859E-04	2.808E-03	7.960E-03	1.911E-02
N O	6.893E-02	7.388E-02	7.082E-02	6.327E-02	5.358E-02
N O2	1.251E-04	9.229E-05	6.039E-05	3.682E-05	2.111E-05
N2 O	3.571E-05	3.929E-05	3.888E-05	3.522E-05	3.077E-05
O	4.501E-02	8.720E-02	1.361E-01	1.825E-01	2.168E-01

TEMP.	H	S	D
1500.	2.893E 01	1.578E 00	2.783E-02
2000.	1.731E 02	1.661E 00	2.086E-02
2500.	3.388E 02	1.734E 00	1.662E-02
3000.	5.645E 02	1.816E 00	1.359E-02
3500.	8.316E 02	1.898E 00	1.132E-02
4000.	1.118E 03	1.975E 00	9.584E-03
4500.	1.458E 03	2.055E 00	8.141E-03
5000.	1.874E 03	2.142E 00	6.894E-03
5500.	2.303E 03	2.224E 00	5.905E-03
6000.	2.675E 03	2.289E 00	5.188E-03

Table 6. Equilibrium Composition, Entropy, Enthalpy, and Density of the Air-Aluminum Gas Mixture Generated in an Exploding Wire Experiment.

PRESSURE = 1000 ATM.

TEMPERATURE	1500	2000	2500	3000	3500
AL2	8.380E-26	4.109E-18	1.653E-13	1.645E-10	1.586E-08
N2	7.895E-01	7.870E-01	7.804E-01	7.653E-01	7.399E-01
O2	1.094E-01	1.070E-01	1.024E-01	9.916E-02	9.712E-02
AL	1.053E-14	3.803E-10	2.053E-07	1.257E-05	1.985E-04
AL O	3.834E-08	1.115E-05	3.248E-04	2.810E-03	1.090E-02
AL2 O	7.540E-07	1.242E-04	2.541E-03	1.596E-02	4.102E-02
AL2 O2	1.000E-01	9.987E-02	9.716E-02	8.164E-02	5.058E-02
N	1.801E-15	2.690E-11	8.719E-09	4.127E-07	6.473E-06
N O	9.480E-04	5.757E-03	1.666E-02	3.348E-02	5.446E-02
N O2	1.031E-04	1.996E-04	2.903E-04	3.709E-04	4.393E-04
N2 O	1.580E-06	8.949E-06	2.578E-05	5.275E-05	8.799E-05
O	4.582E-08	7.489E-06	1.589E-04	1.223E-03	5.273E-03

TEMPERATURE	4000	4500	5000	5500	6000
AL2	3.564E-07	3.389E-06	1.849E-05	6.490E-05	1.502E-04
N2	7.127E-01	6.880E-01	6.640E-01	6.379E-01	6.092E-01
O2	8.863E-02	7.316E-02	5.582E-02	4.076E-02	2.937E-02
AL	1.344E-03	5.468E-03	1.594E-02	3.579E-02	6.334E-02
AL O	2.466E-02	4.009E-02	5.272E-02	5.875E-02	5.598E-02
AL2 O	5.806E-02	6.004E-02	5.198E-02	3.835E-02	2.327E-02
AL2 O2	2.394E-02	1.001E-02	3.979E-03	1.488E-03	4.976E-04
N	5.098E-05	2.544E-04	9.217E-04	2.641E-03	6.342E-03
N O	7.486E-02	8.974E-02	9.725E-02	9.837E-02	9.532E-02
N O2	4.597E-04	4.205E-04	3.468E-04	2.682E-04	2.013E-04
N2 O	1.246E-04	1.546E-04	1.754E-04	1.818E-04	1.818E-04
O	1.522E-02	3.269E-02	5.688E-02	8.546E-02	1.162E-01

TEMP.	H	S	D
1500.	2.895E 01	1.444E 00	2.783E-01
2000.	1.726E 02	1.527E 00	2.087E-01
2500.	3.280E 02	1.596E 00	1.667E-01
3000.	5.144E 02	1.664E 00	1.378E-01
3500.	7.438E 02	1.734E 00	1.158E-01
4000.	9.888E 02	1.800E 00	9.912E-02
4500.	1.238E 03	1.858E 00	8.610E-02
5000.	1.504E 03	1.915E 00	7.538E-02
5500.	1.806E 03	1.972E 00	6.616E-02
6000.	2.147E 03	2.031E 00	5.814E-02

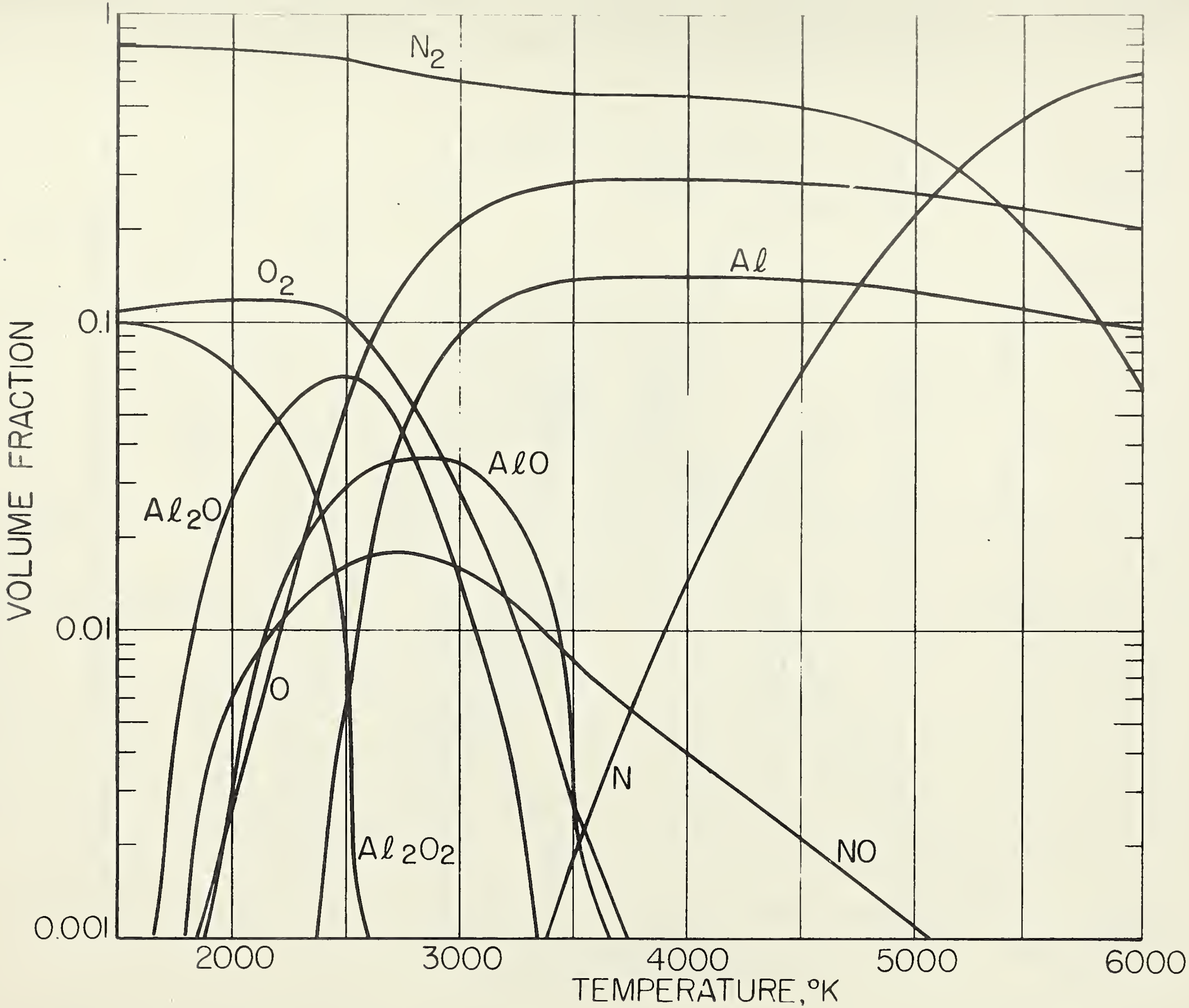

Figure 1. Equilibrium Concentrations of the Various Components in the Explosion Mixture for p = 0.01 atm.

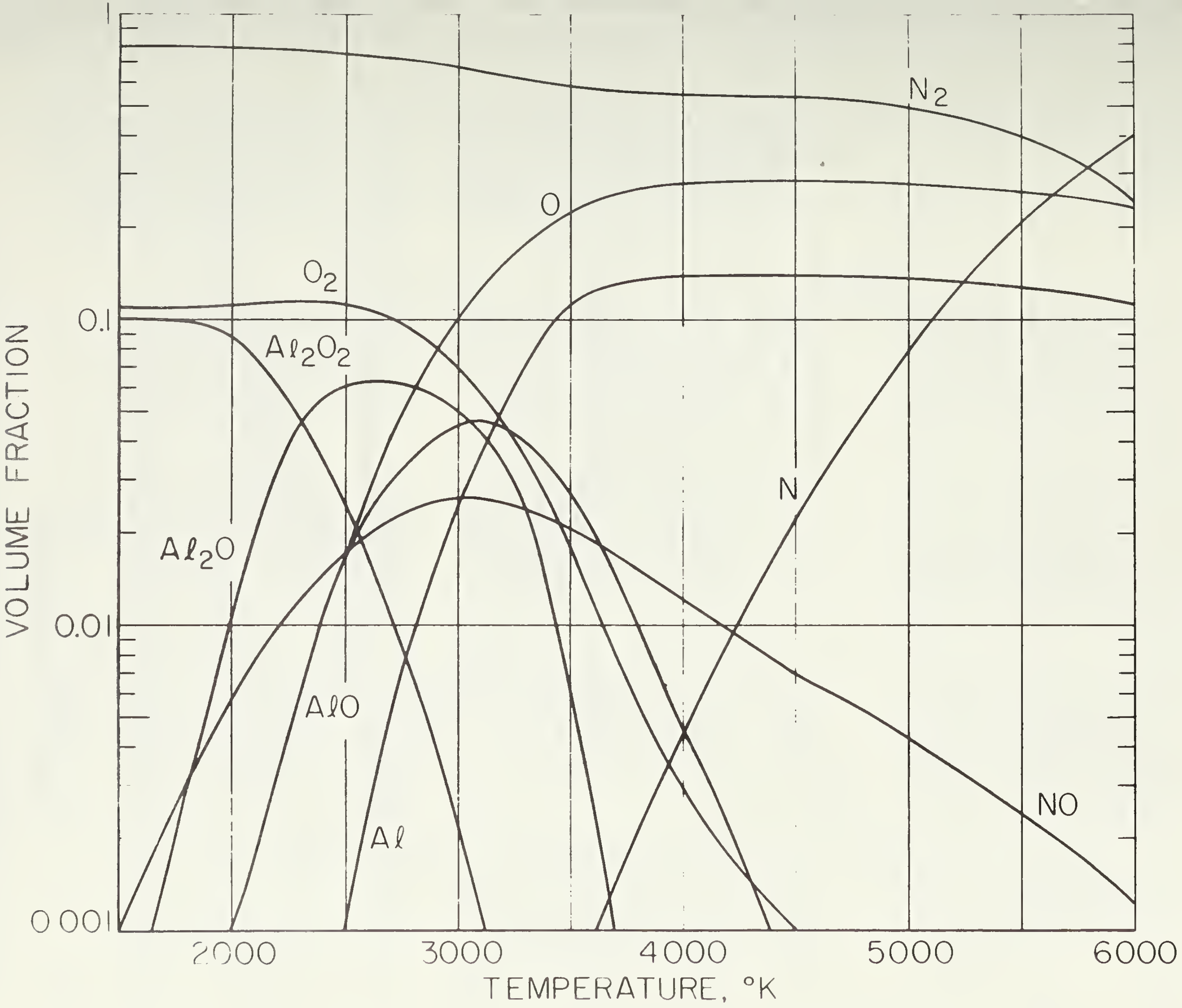

Figure 2. Equilibrium Concentrations of the Various Components in the Explosion Mixture for $p = 0.1$ atm.

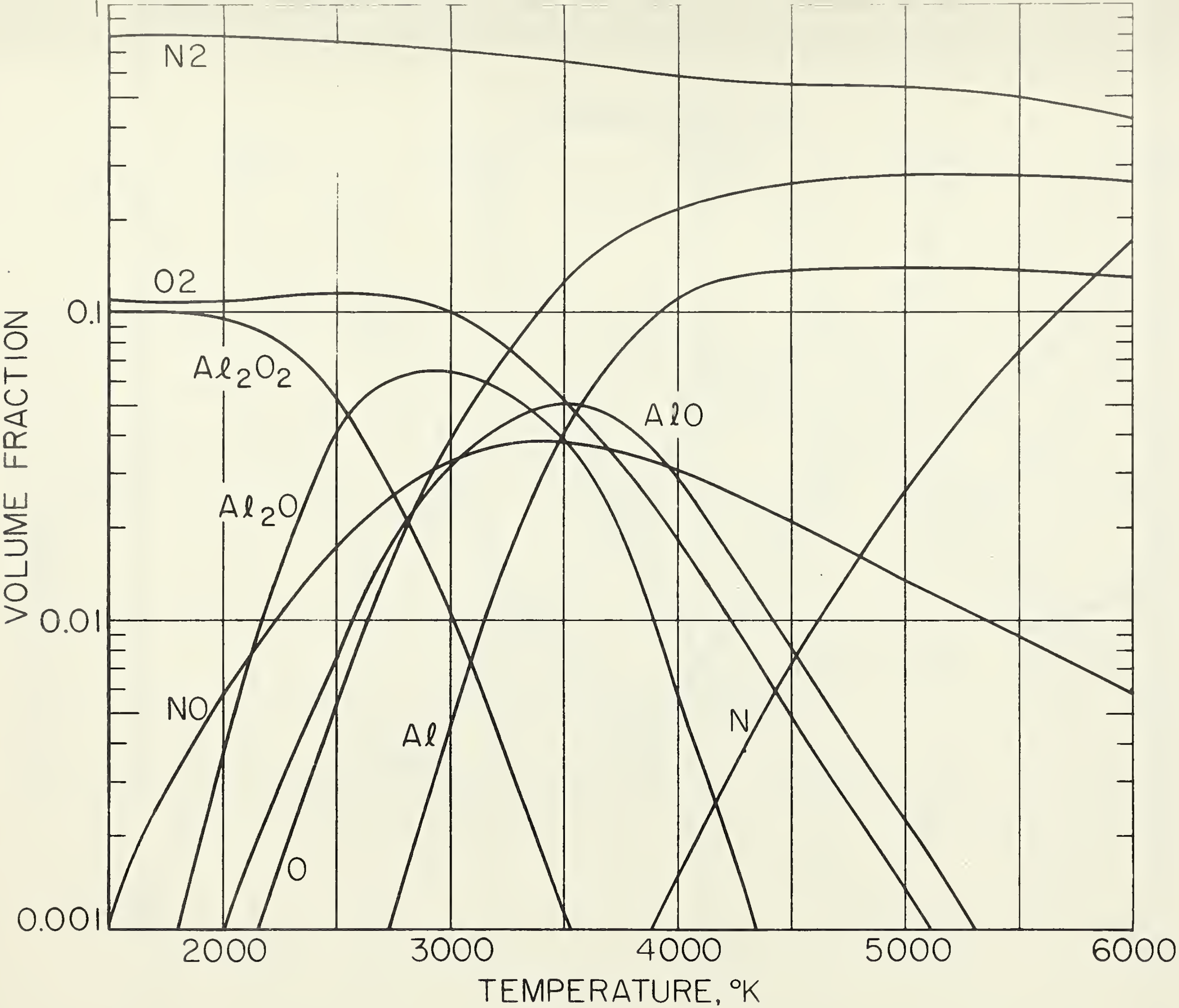

Figure 3. Equilibrium Concentrations of the Various Components in the Explosion Mixture for p = 1 atm.

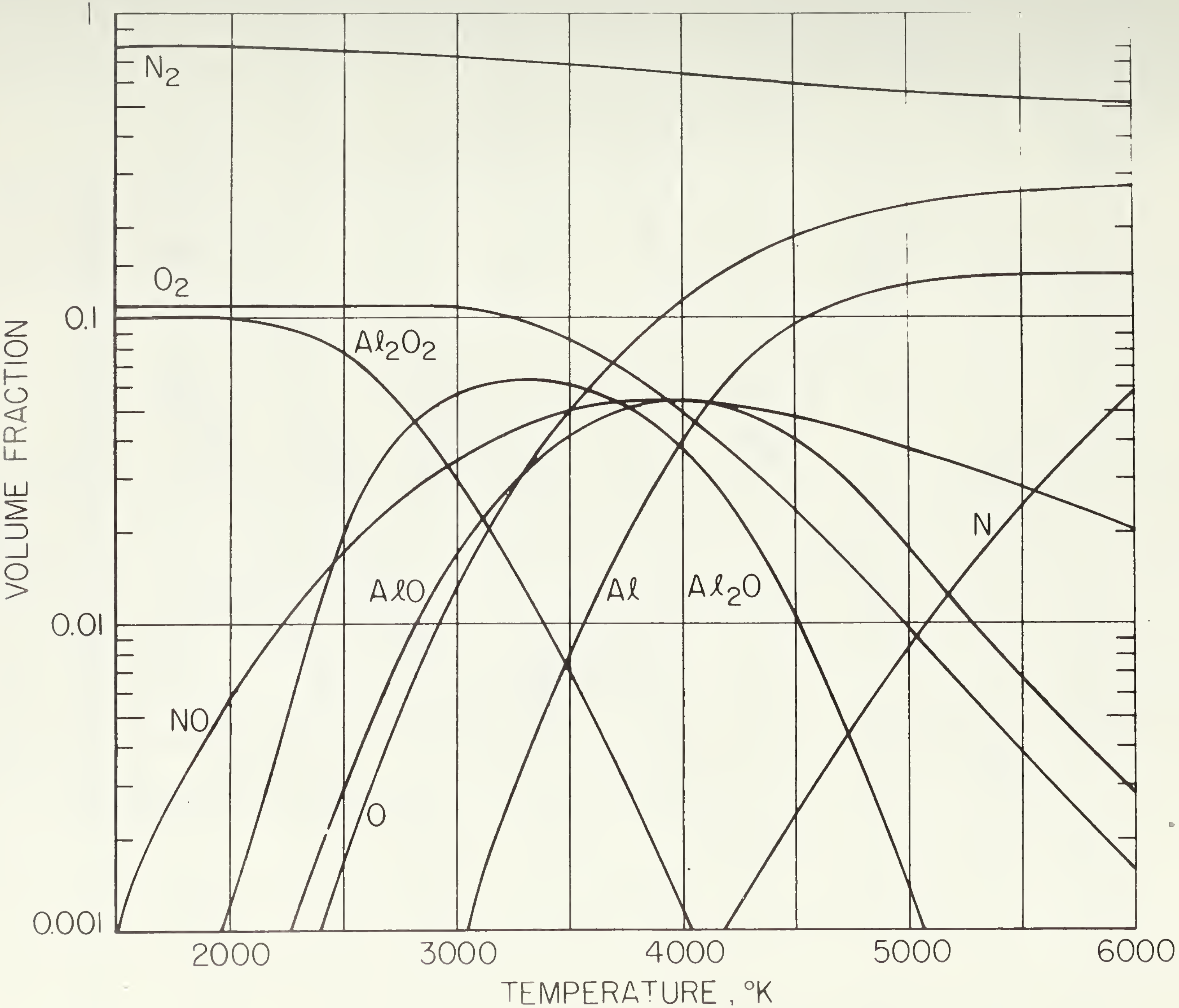

Figure 4. Equilibrium Concentrations of the Various Components in the Explosion Mixture for $p = 10$ atm.

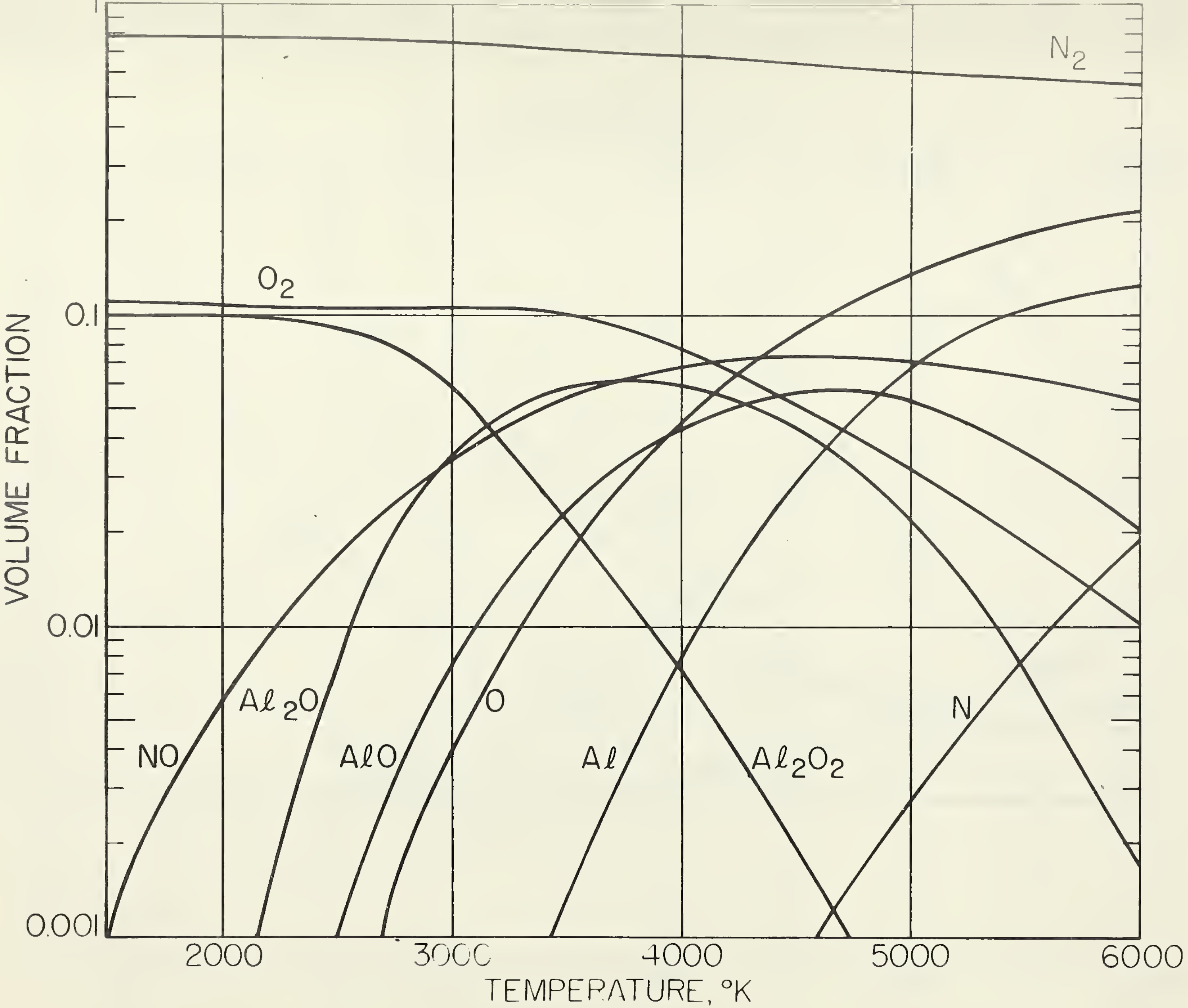

Figure 5. Equilibrium Concentrations of the Various Components in the Explosion Mixture for p = 100 atm.

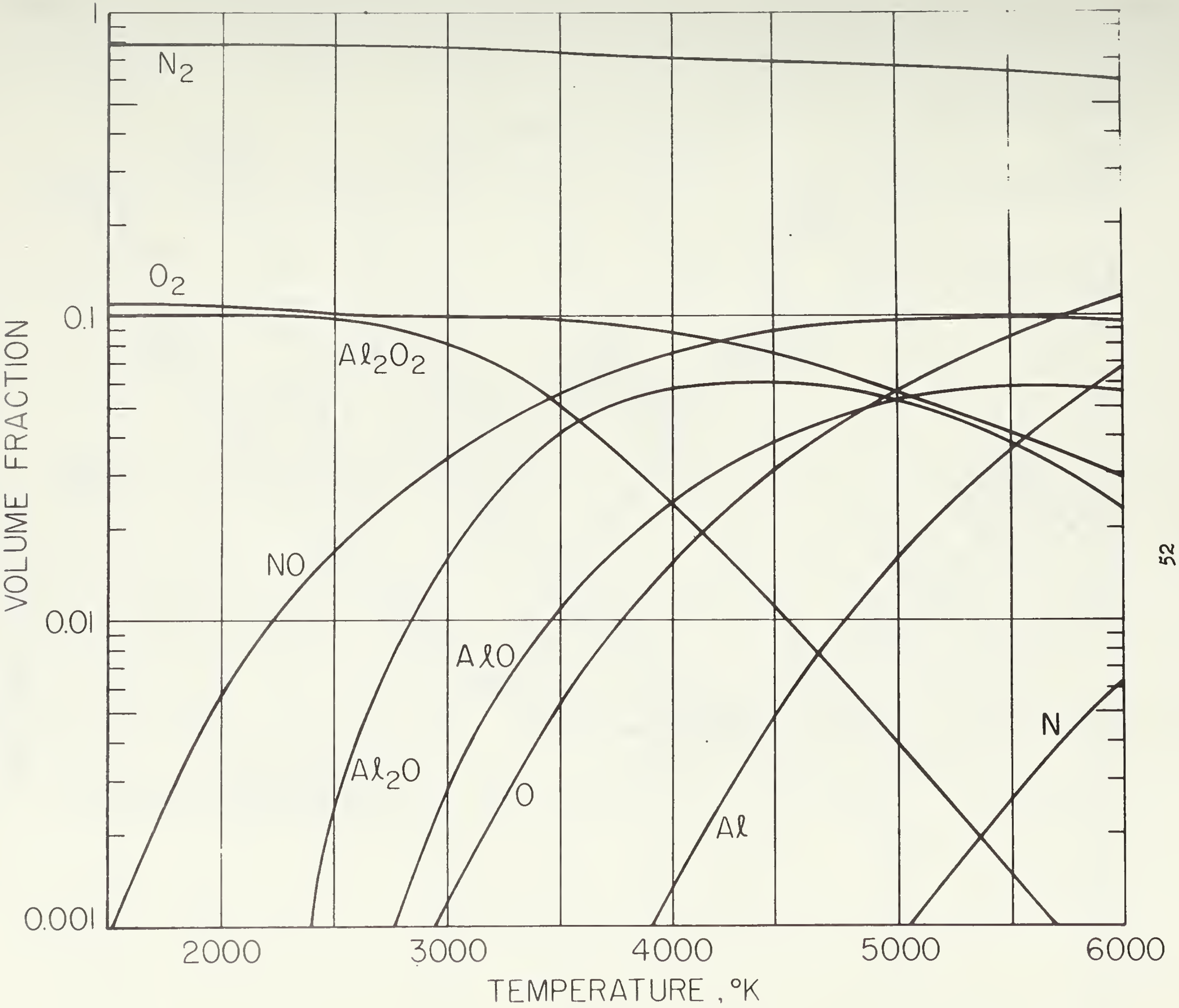

Figure 6. Equilibrium Concentrations of the Various Components in the Explosion Mixture for p = 1000 atm.

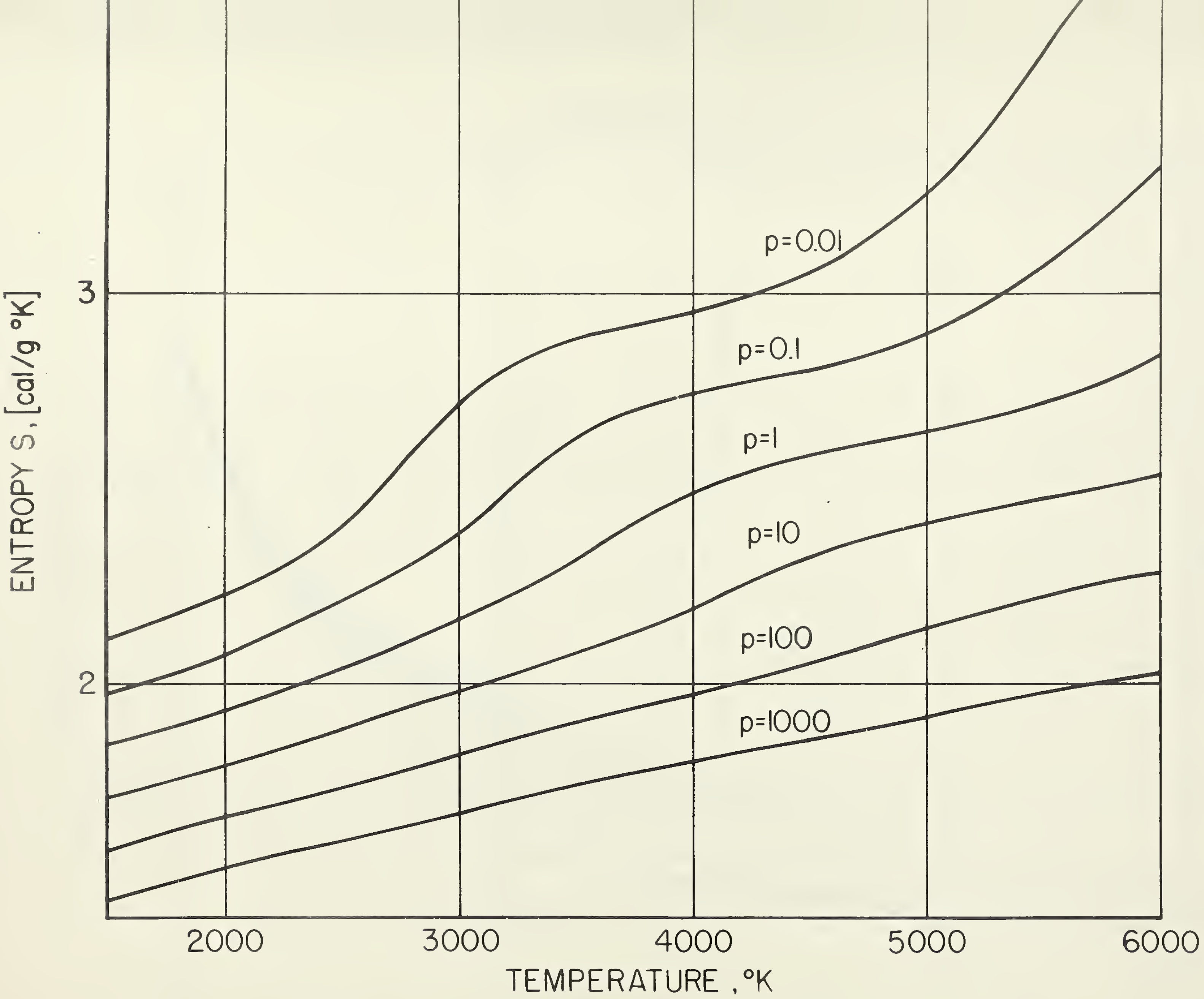

Figure 7. Entropy Diagram for the Explosion Mixture.

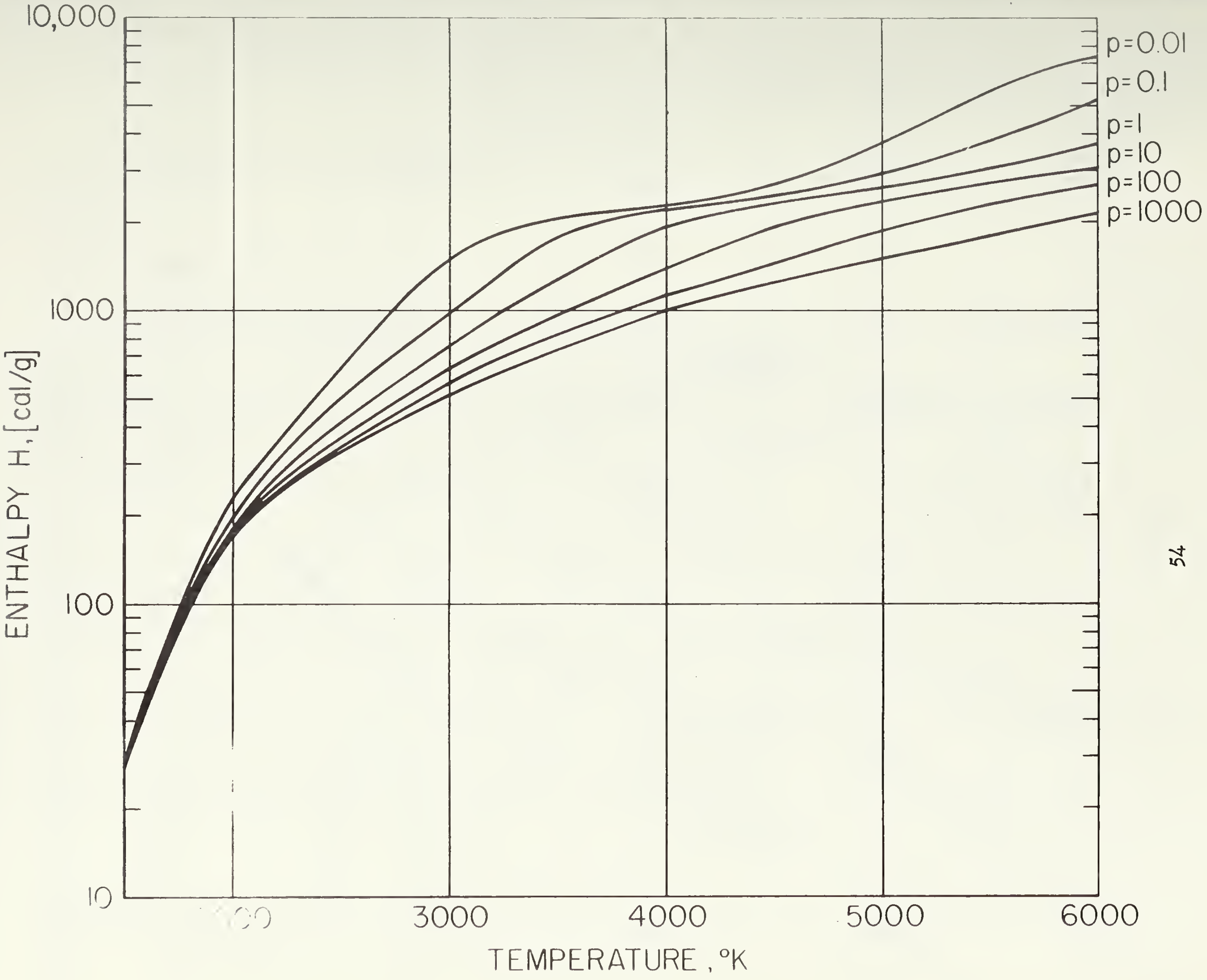

Figure 8. Enthalpy Diagram for the Explosion Mixture.

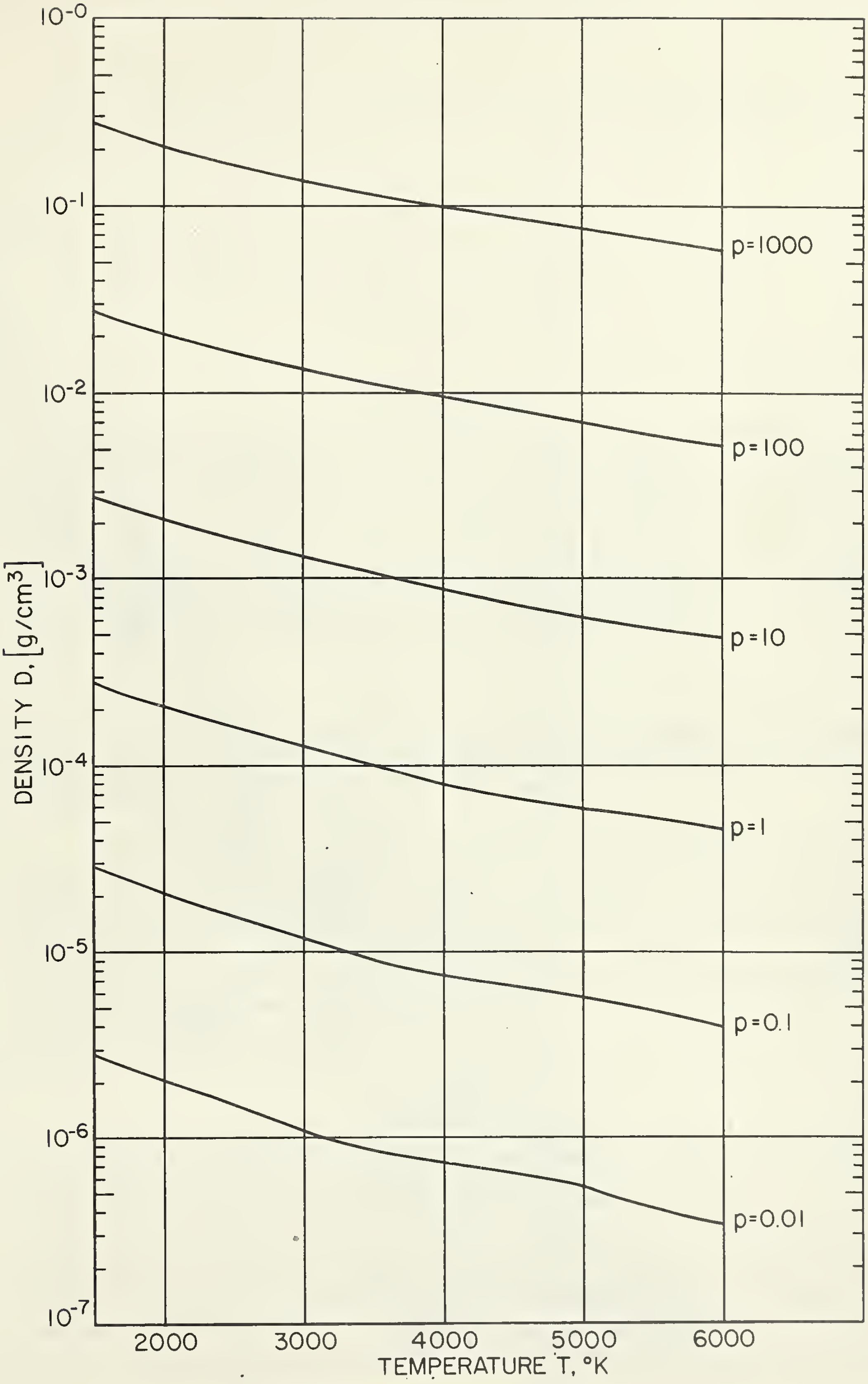

Figure 9. Density Diagram for the Explosion Mixture.

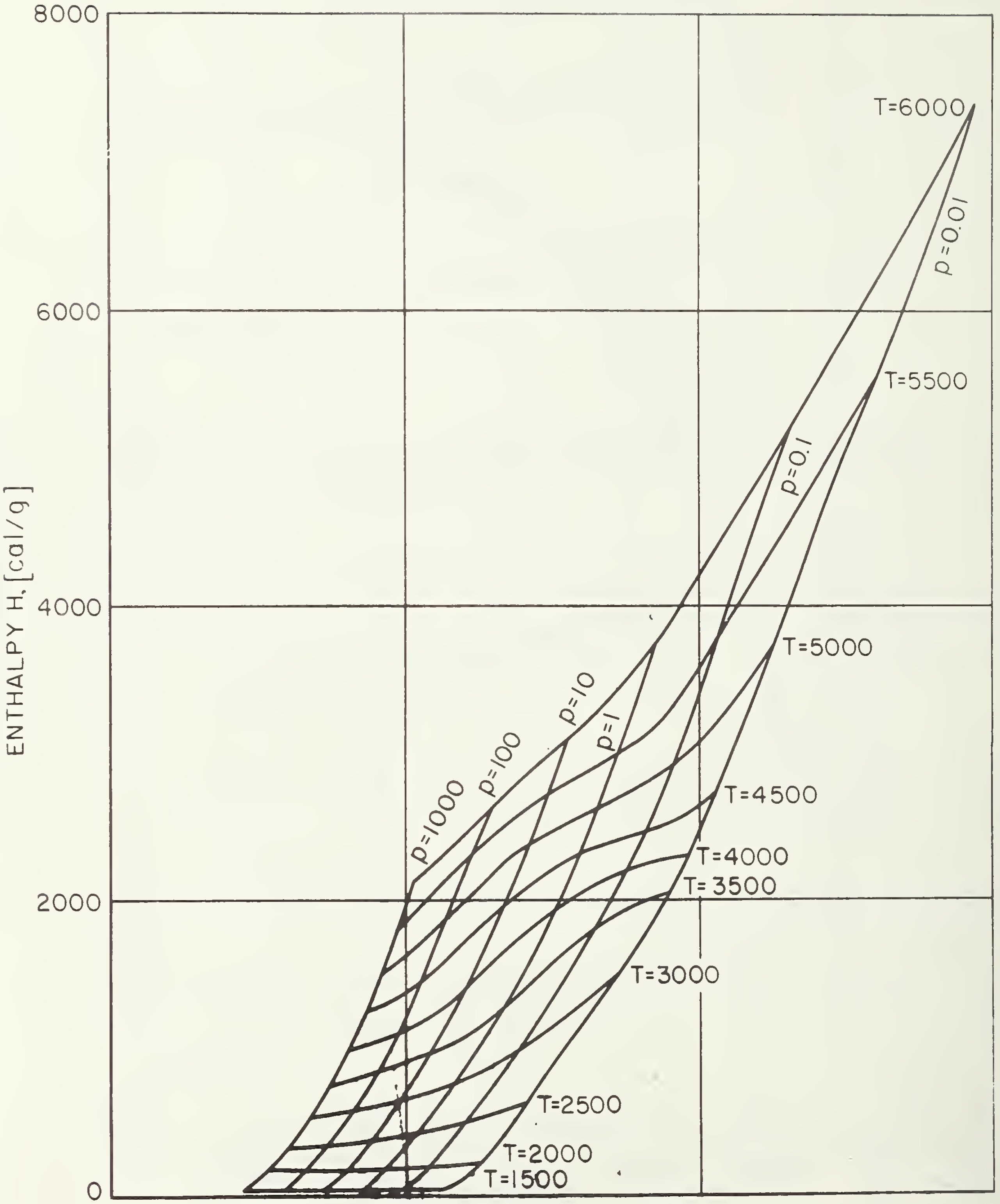

Figure 10. Entropy-Enthalpy Diagram for the Explosion Mixture.

Chapter B-4

HIGH TEMPERATURE MICROWAVE SPECTROSCOPY: AlF and AlCl

by David R. Lide, Jr.

Introduction

The first evidence for the existence of the monohalides of aluminum came from emission spectra. Band systems of both AlCl (1,2) and AlF (3) were identified in emission from discharges through the corresponding trihalide. Bands were later observed in absorption (4,5) by heating the trihalides in a reducing environment, which indicated that the monohalide species were relatively unreactive. The physical chemistry of AlCl and AlF was investigated by Gross and coworkers (6,7). They studied the thermodynamics of reactions such as

$$AlX_3 + 2Al \rightleftarrows 3AlX$$

and from the results were able to estimate the dissociation energy of AlCl and AlF. Large concentrations of both species were achieved at temperatures in the neighborhood of 1000°C.

The above evidence suggested that conditions might exist under which microwave absorption spectra of the aluminum monohalides could be detected. Calculations using the best estimates of the thermodynamic properties of the species involved indicated that reasonably high concentrations of the monohalides should be attainable at pressures of the order of 10-100 μ Hg and temperatures in the range 600-800°C. The predictions were confirmed, and microwave transitions of both AlF and AlCl were observed and analyzed.

Experimental

The spectrometer used in this investigation has been briefly described (8), but some further details may be useful. A diagram of the high-temperature waveguide assembly is given in Fig. 1. The vacuum jacket is a quartz tube of about 42 mm I.D. and 120 cm length; it is inserted into a brass sleeve at each end and sealed with Apiezon W wax. Brass flanges are attached by rubber O-rings to each sleeve, and 0.001 in. mica windows are waxed to these flanges. The system can thus be easily opened for cleaning and sample admission.

The waveguide is made of stainless steel and is approximately 150 cm long. The cross-section is illustrated in Fig. 2. The guide is of a type (9) which is very useful for high temperature operation; it is fed such that the microwave electric field is vertical (Fig. 2), while the Stark modulation field is applied horizontally between the two halves. In the present apparatus the inside dimensions are about 6×24 mm. This choice gives satisfactory homogeniety of the Stark field and leads to a cutoff frequency of 25 Gc. Lower-frequency operation is possible by increasing the smaller dimension, at a slight sacrifice of Stark homogeniety. The guide is held together by 1 cm mica strips screwed into top and bottom at 15 cm intervals in the cool regions. For added rigidity ceramic spacers may be added in the hot region, although these are often unnecessary. This type of waveguide has been found to give satisfactory broad-banded operation at frequencies up to 60 or 70 Gc and can probably be used even higher.

The central region of about 50 cm length is heated by a simple tube furnace (Fig. 1). The conductivity of the quartz and stainless steel is sufficiently low that the center can be maintained at 1000°C while the brass sleeves remain close to room temperature. Blowers are used when necessary for cooling the ends. The depth of insertion of the quartz tube into the brass sleeves is empirically adjusted to leave a suitable gap at room temperature between the waveguide ends and the mica windows which will roughly compensate for the differential thermal expansion. This adjustment is not very critical, since a residual gap of 1 or 2 mm at the windows does not cause a serious mis-match.

In studying the spectrum of a simple volatile material the sample is placed in a tray in the hot zone (Fig. 2), and, after thorough outgassing, the system is heated to a temperature which will give a suitable vapor pressure (1 to 50 μ Hg). The vapor diffuses into the waveguide through the slot and condenses in the cooler regions outside the furnace zone. We thus have a crude flow system with an effective path length of perhaps 30-50 cm. In the work reported here it was necessary to generate the aluminum monohalides in situ by reduction of the trihalides. This was readily done for AlF by placing a mixture of AlF_3 and powdered Al in the sample tray. The reaction was found to proceed well enough at 600-700°C to give sufficient AlF vapor for spectroscopic purposes. This reaction is a very convenient one because both AlF_3 and Al have completely negligible vapor pressures at these temperatures. The chloride system, on the other hand, is not so clean because of the high volatility of $AlCl_3$. Here it was necessary to have a separate reservoir of $AlCl_3$ outside the furnace zone, while the sample tray was filled with powdered Al. The $AlCl_3$ was heated to about 75°C and the vapor conducted through a small quartz tube into the hot zone, where it reacted with the solid or liquid aluminum.

In the simplest style of operation the high-temperature cell is pumped continuously with a high-speed diffusion pump. This is necessary in cases where sample decomposition occurs or where outgassing is difficult to eliminate. However, when static operation is possible, a significant improvement in sensitivity can be achieved by adding a small amount of helium as a buffer gas. This retards diffusion of the sample vapor and thus leads to a higher partial pressure and longer effective path. The expected loss of absorption intensity from sample dilution is partially compensated by the much smaller collision broadening parameter in the helium mixture, so that a net gain of intensity results. This is illustrated in Fig. 3 for the $J = 0 \rightarrow 1$ transition of AlF. It is seen that the peak intensity is greatly increased without an excessive increase in line width when 0.2 mm Hg of helium is added.

The microwave spectrometer itself was a conventional 80 kc Stark-modulation instrument. Klystrons were used as sources, and frequency measurements were made by comparison with the NBS standard frequency.

Observed Spectra and Rotational Constants

The $J = 0 \rightarrow 1$ transition of AlF was observed in the $v = 0$ and $v = 1$ states; frequencies are listed in Table I and the spectrum is illustrated in Fig. 3. In AlCl the $J = 1 \rightarrow 2$ transition was measured for the ground state of $AlCl^{35}$, and the $J = 2 \rightarrow 3$ transition for the $v = 0$ and $v = 1$ states of $AlCl^{35}$ and the $v = 0$ state of $AlCl^{37}$. The major observed lines are listed in Table II. The assignments were confirmed by Stark effects, hyperfine structure, and the general spectral pattern.

After the reduction of the nuclear quadrupole hyperfine structure, which is discussed below, the hypothetical unshifted frequencies were used to calculate rotational constants in the usual manner. Calculated values of the centrifugal distortion constant D_e were used in the data reduction. These were obtained from the relation $D_e = 4B_e^3/\omega_e^2$ with (1-5) $\omega_e = 814\ cm^{-1}$ for AlF and $481\ cm^{-1}$ for AlCl. The final constants are collected in Table III.

Rotational constants reported previously from optical spectra do not differ greatly from the more accurate values obtained here. In AlF our value of $0.552467\ cm^{-1}$ for B_e compares with $0.5523\ cm^{-1}$ given by Naude and Hugo (10). For $AlCl^{35}$ we obtain $B_e = 0.24393\ cm^{-1}$, while the optical value (2) is $0.242\ cm^{-1}$.

Nuclear Quadrupole Hyperfine Structure

The J = 0 → 1 transition of AlF shows a simple triplet structure (Fig. 3) characteristic of a single quadrupolar nucleus. The spacings and relative intensities indicate I = 5/2, in agreement with the known spin of Al^{27}. The resulting quadrupole coupling constant is -37.6±1.0 Mc.

The hyperfine structure in AlCl is much more complicated. The interaction of two nuclei of spins 5/2 and 3/2 with the molecular rotation produces a very complex pattern which could be only partially resolved in this work. For the J = 1 → 2 and 2 → 3 transitions the bulk of the intensity is concentrated in a strong central peak. However, some outlying weaker features could be detected, and in the J = 1 → 2 transition the central peak could be partially resolved (Fig. 4).

The calculation of the hyperfine pattern was rather tedious because the coupling constants of Al^{27} and Cl^{35} are too close in magnitude for first-order approximations to be valid. The procedure followed the outline of Townes and Schawlow (12). The Al spin of 5/2 was coupled with J to give an intermediate quantum number F_1; this was in turn coupled with the chlorine spin of 3/2 to give the total angular momentum quantum number F. The energy matrix was set up in an F_1F representation. The transformation matrices needed to express the chlorine quadrupolar energy in this representation were calculated from Rotenberg's tabulation of 6j coefficients (12). The quadrupole energy matrix factors into six submatrices for J = 1, seven for J = 2, and eight for J = 3; the largest of these are 4X4.

The factored matrices were diagonalized by computer for various ratios of the coupling constants. A satisfactory fit of the observed pattern could be obtained only for a ratio of Cl to Al in the neighborhood of 0.30. The resulting coupling constants are -29.2±2.0 Mc for Al^{27} and -8.8±1.5 Mc for Cl^{35}. The patterns calculated from these constants are compared with the observed spectrum in Fig. 4. Only the strongest of the calculated hyperfine components are included here; the total number of allowed components amounts to several hundred. The observed and calculated frequencies in the J = 1→ 2 transition are listed in Table IV.

The quadrupole coupling constant of Al in both AlF and AlCl is close to that in the free aluminum atom (-37.5 Mc). When this fact is coupled with the relatively small dipole moments of 1 to 2 D (see next section), one might be tempted to conclude that the aluminum-halogen bond is predominately covalent in character. However, this interpretation is probably misleading. If the bonds were purely ionic, and if the two remaining valence electrons of the Al atom were in the 3s orbital, then one would predict dipole moments er_e = 7.9 D in AlF and 10.2 in AlCl (ignoring polarization effects). However, a more realistic starting point is an Al atom with a promoted s electron so that sp hybrid orbitals can be formed; then the electron which is to form the bond is placed in the s + pσ orbital, while the two remaining electrons form a lone pair in the s-pσ orbital on the opposite side of the Al nucleus (13). Now even is the bond to the halogen atom is highly ionic, the bond dipole moment will be opposed by the rather large moment from the lone pair, and a small net moment could easily result. A rather analogous situation is suggested by theoretical calculations on the hydrides of the first and second row elements (14). The calculated dipole moment of NaH is 6.6 D with the H negative, while that for AlH is 0.7 D with the H positive.

The quadrupole coupling constants of Al are also consistent with an ionic bond. Since the ground state of the Al atom is derived from the configuration $3s^2 3p$, we may reasonably identify the atomic eq Q as the coupling from a single 3p electron. In the bonding picture discussed above, the lone pair in an s-pσ orbital would contribute to eq Q the same amount as a single p electron. Thus the fact that eq Q of Al is roughly the same in the molecule as in the atom suggests that the electron in the bond makes little contribution, - i.e., that the bond is largely ionic. This suggestion is reinforced when we consider eq Q of Cl^{35} in AlCl. This is only -8.8 Mc, which may be compared with -110 Mc in the free atom and -60 to -80 Mc in organic chlorides which are considered typical examples of covalent binding.

It would be interesting to place these rather crude ideas on a quantitative basis. However, all of the present evidence seems to suggest that the AlF and AlCl bonds show a large degree of ionic character.

Stark Effect

It has been pointed out that the selection rule on the Stark effect is $\Delta M = \pm 1$ in the present apparatus. This selection rule, coupled with the quadrupole hyperfine structure, led to quite complicated Stark patterns. In AlF it was still possible to resolve several well-defined components. Quantitative measurements on AlF are illustrated in Fig. 5. The observed points fall in the intermediate field region, so that it was necessary to carry out exact calculations of the Stark-quadrupole energy. The electric field strength was calibrated by making Stark measurements on LiCl, whose dipole moment is accurately known (8), at the same temperature of the AlF measurements. This procedure was necessary because the waveguide spacing was found to change by about 10% upon heating from room temperature to 600°C. The measurements on AlF resulted in a dipole moment of 1.53 ± 0.10 D.

The hyperfine structure in AlCl is too complex for any detailed study of the Stark effect. However, a rough indication of the dipole moment may be obtained from the magnitude of the Stark field required to bring the observed lines to full intensity. On this basis we can say that the dipole moment of AlCl is very probably in the range 1 to 2 D, and therefore is comparable in magnitude to that of AlF.

Thermodynamic Considerations

The conditions required for the observation of the microwave spectra of AlF and AlCl provide some information on the equilibrium constants of the reactions used to generate the monohalides. Since the thermodynamic properties of the trihalides and of aluminum itself are known with reasonable accuracy, we may in principle use this information to estimate the heat of formation of the monohalides. Fig. 6 shows a plot of the temperature required to produce a given partial pressure of AlF *vs*. the assumed ΔH_f^o of AlF. The minimum pressure necessary for detection of AlF lines is difficult to specify accurately but is probably not far from the 1 - 10 μ Hg range. Since the AlF lines were found to appear quite reproducibly when the temperature reached 620°C, we obtain from Fig. 6 an estimate of -60 to -64 kcal/mole for ΔH_f^o of AlF. This is in excellent agreement with the most widely accepted value (-61 kcal/mole) (7,15).

The situation in AlCl is not as simple because the initial pressure of $AlCl_3$ was not accurately known. However, the temperature at which the AlCl spectrum first appeared (650-700°C) is consistent with the accepted value (6) of -11 kcal/mole for ΔH_f^o of AlCl.

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Table I. Observed spectrum of AlF.

Transition	F → F'	Freq. (v = 0)	Freq. (v = 1)
J = 0 → 1	5/2 → 5/2	32970.6±0.1 Mc	32673.9±0.1
	5/2 → 7/2	32978.5	32681.6
	5/2 → 3/2	32981.8	...

Table II. Observed spectrum of AlCl.

Species	State	Transition	Obs. ν^a	ν_o^b
$Al^{27}Cl^{35}$	v = 0	J = 1 → 2	29155.6±0.2	29154.8
	v = 0	J = 2 → 3	43731.8±0.2	43731.5
	v = 1	J = 2 → 3	43443.7±0.2	43443.4
$Al^{27}Cl^{37}$	v = 0	J = 2 → 3	42704.6±0.2	42704.3

[a] Frequency of strong central peak; see Fig. 4 for detailed pattern.

[b] Hypothetical unshifted frequency after correction for hyperfine structure.

Table III. Constants for AlCl and AlF.

	$Al^{27}Cl^{35}$	$Al^{27}Cl^{37}$	$Al^{27}F^{19}$
B_0	7288.73±0.04 Mc	7117.52±0.04 Mc	16488.36±0.05 Mc
B_1	7240.70±0.04	...	16339.96±0.05
D_e	0.0075[a]	0.0072[a]	0.030[a]
B_e	7312.74±0.06	7140.69±0.06	16562.56±0.10
α_e	48.03±0.06	46.34[a]	148.40±0.10
$(eqQ)Al^{27}$	-29.2±2.0	...	-37.6±1.0
$(eqQ)Cl^{35}$	-8.8±1.5	...	...
r_e	2.12983±0.00001 Å[b]	2.12983±0.00001 Å[b]	1.65437±0.00001 Å[b]
μ	~1-2 D	...	1.53±0.10 D

[a] Calculated from theoretical relations.

[b] Includes only the experimental uncertainty. Because of the uncertainty in the atomic constants plus the neglect of higher order terms in the theory, the absolute accuracy of r_e is about ±0.0001 Å. The constants used were: $h = 6.6256\times10^{-27}$ erg sec, $N_A = 6.2252\times10^{23}$ mol^{-1}, $m(Al^{27}) = 26.99014$, $m(Cl^{35}) = 34.97993$, $m(Cl^{37}) = 36.99754$.

Table IV. Hyperfine structure[a] of $J = 1 \rightarrow 2$, $v = 0$, transition of $Al^{27}Cl^{35}$ (in Mc).

$F_1 \rightarrow F_1'$	$F \rightarrow F'$	Calc. ν	Obs. ν
3/2 → 5/2	3 → 4	29147.84	29148.5±0.2
3/2 → 5/2	2 → 3	148.70	
7/2 → 7/2	2 → 2	148.70	
7/2 → 7/2	5 → 5	149.31	
3/2 → 3/2	3 → 3	151.83	151.7
5/2 → 7/2	3 → 4	154.30	154.1
7/2 → 9/2	4 → 5	155.21	155.33
5/2 → 7/2	2 → 3	155.56	155.69
7/2 → 9/2	5 → 6	155.63	
7/2 → 9/2	3 → 4	155.99	156.18
7/2 → 9/2	2 → 3	156.16	
5/2 → 7/2	4 → 5	156.55	156.7
5/2 → 5/2	4 → 4	158.15	158.0
5/2 → 3/2	2 → 1	161.38	161.5
5/2 → 3/2	3 → 2	161.56	
5/2 → 3/2	4 → 3	162.11	162.1

[a] Only the stronger components of the calculated pattern are listed.

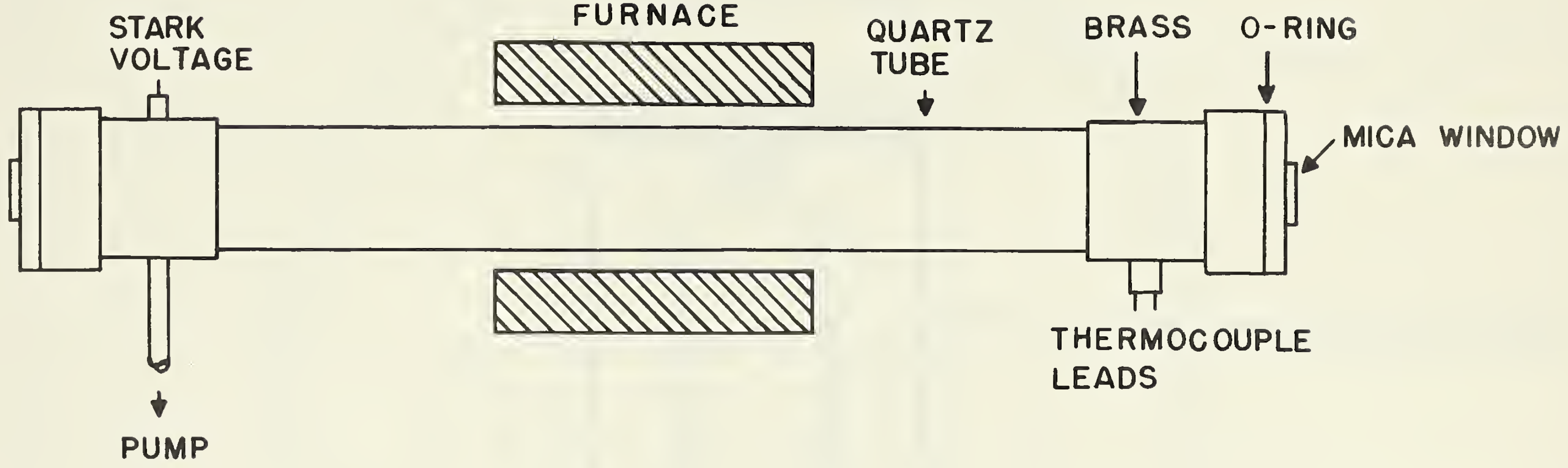

Fig. 1 - Diagram of high-temperature waveguide assembly.

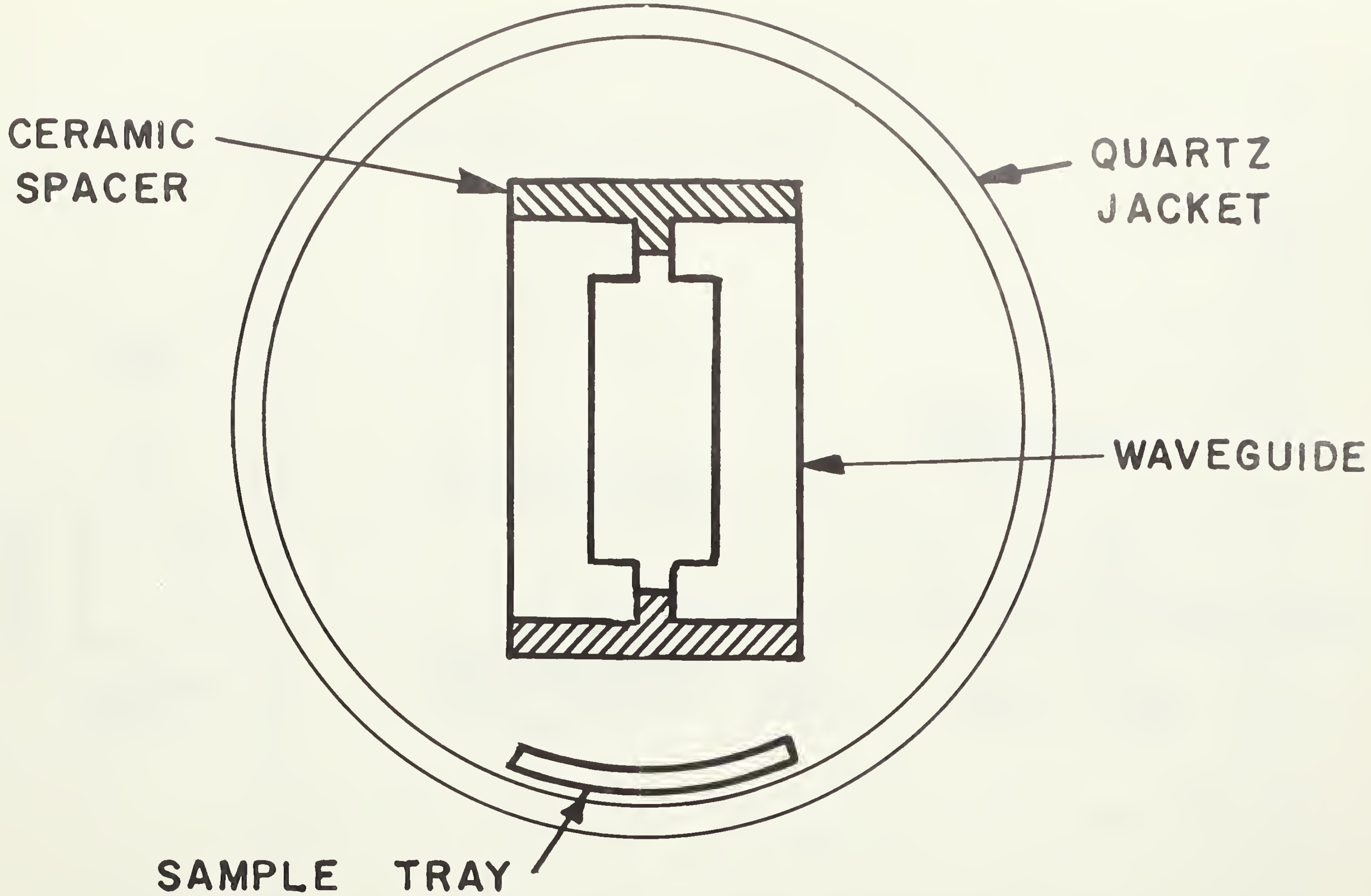

Fig. 2 - Cross-section of waveguide.

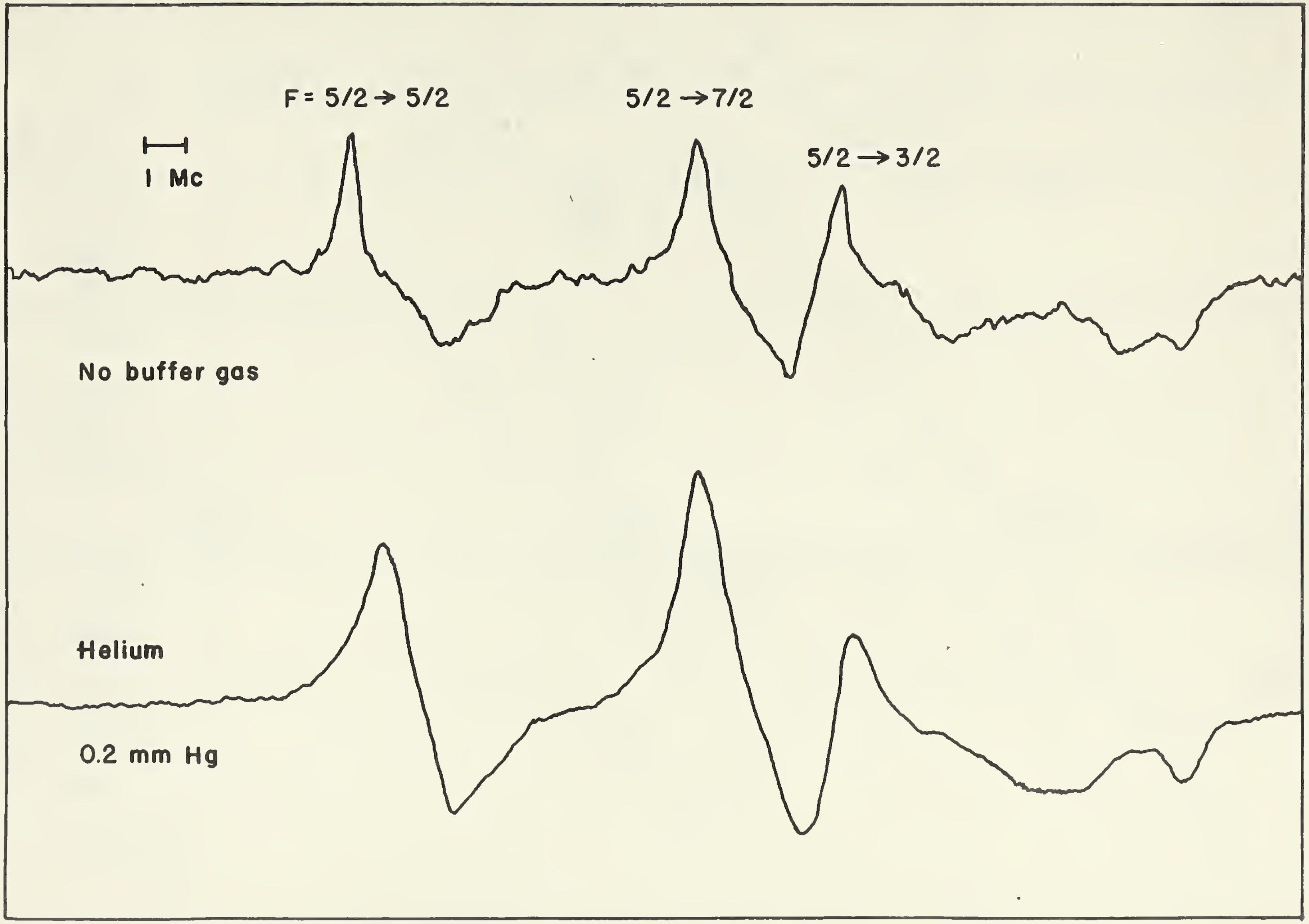

Fig. 3 - Recorder traces of the $J = 0 \rightarrow 1$, $v = 0$, transition of AlF near 33000 Mc. In the lower trace the gain has been reduced by a factor of three.

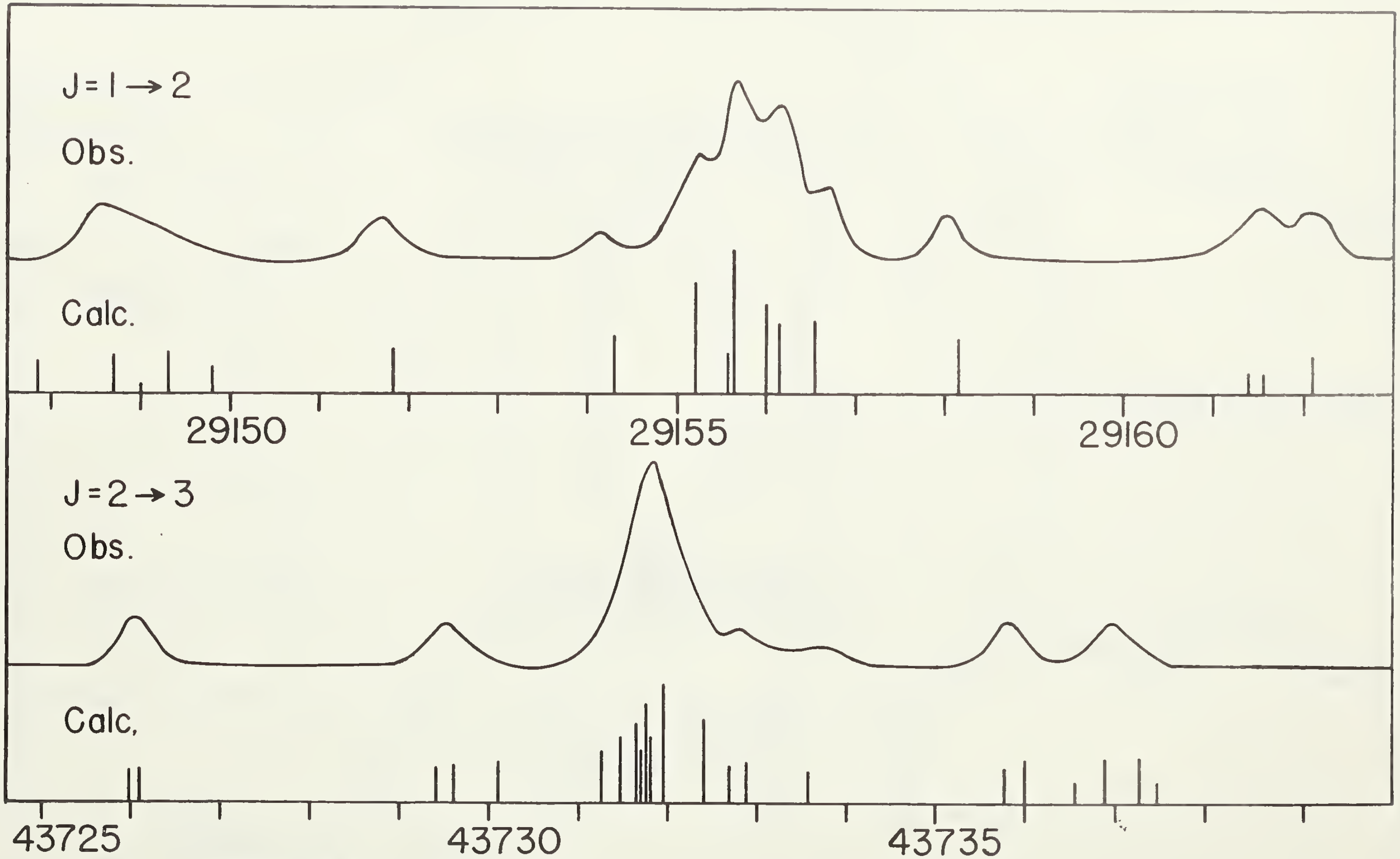

Fig. 4 - Observed and calculated hyperfine patterns in AlCl. Only the stronger of the calculated components are included, and the intensities are approximate.

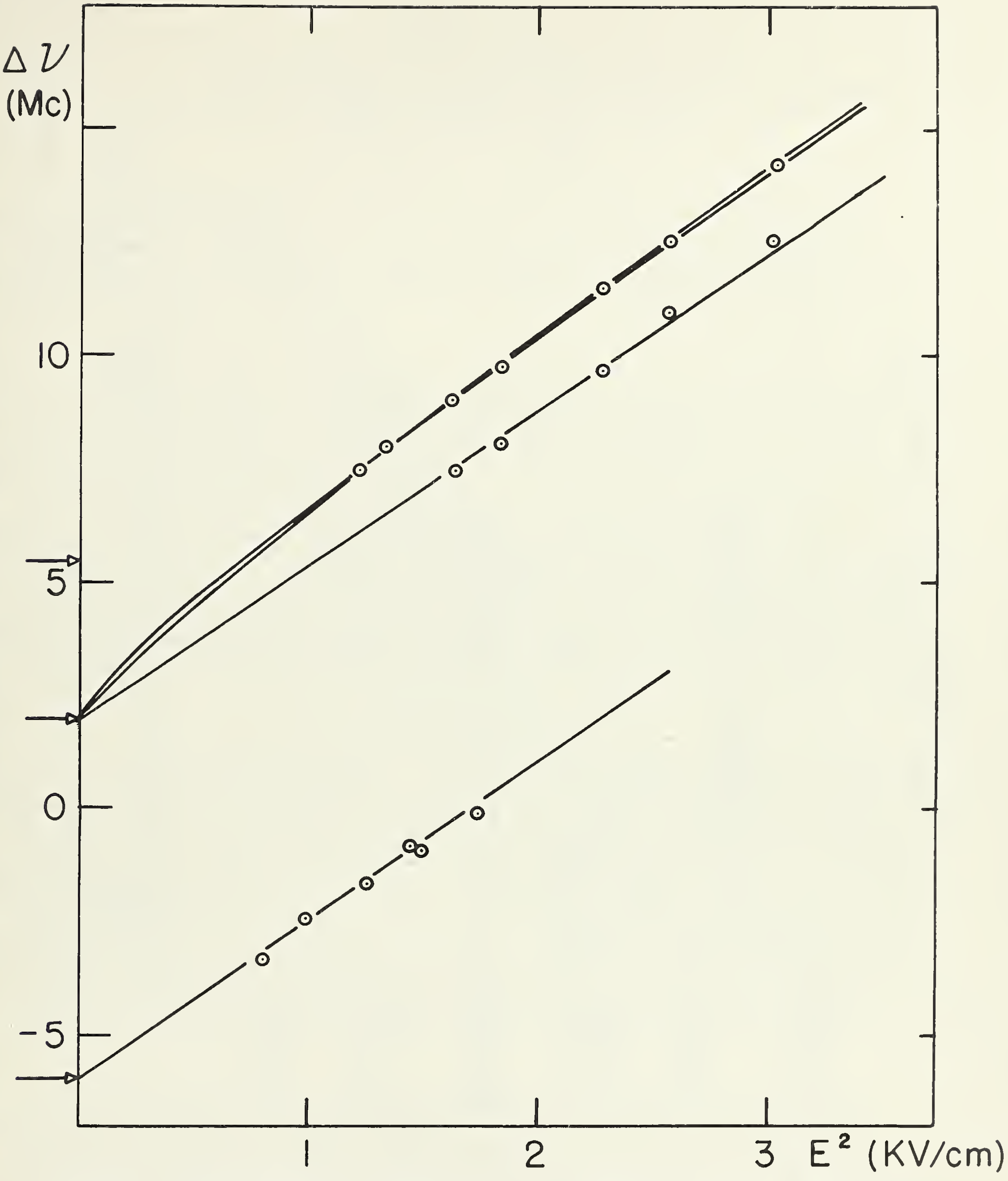

Fig. 5 - Stark effect of the J = 0 → 1 transition of AlF. The zero of the frequency scale is at ν_0 = 32976.6 Mc. The curves are calculated for a dipole moment of 1.53 D.

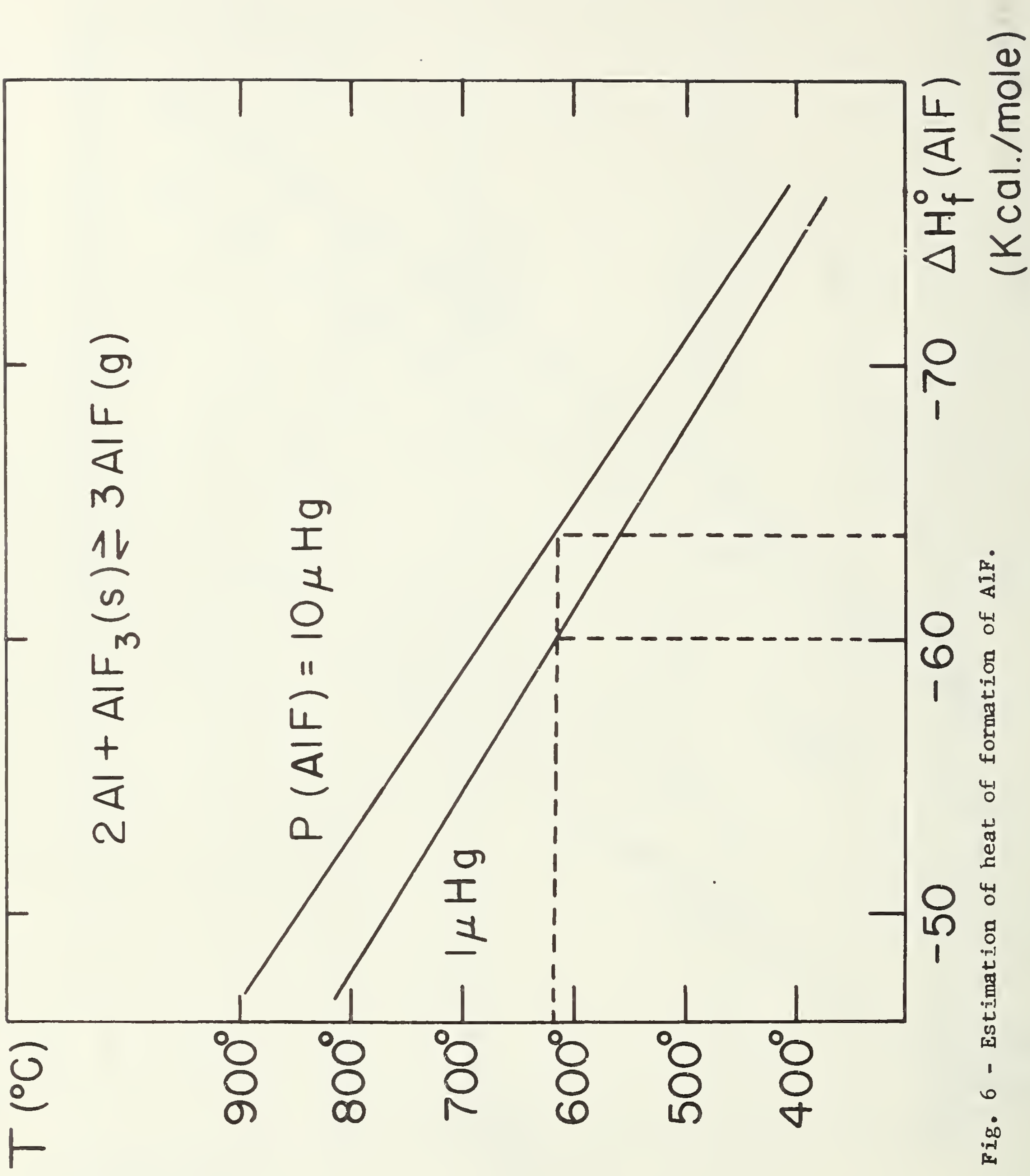

Fig. 6 - Estimation of heat of formation of AlF.

Chapter B-5

APPARATUS FOR HIGH TEMPERATURE PREPARATION OF PURE CRYSTALLINE POLYMORPHS

by Augustus R. Glasgow, Jr.

This research was undertaken to extend phase purifications and separations to 1000°C for the preparation of pure crystalline forms of polymorphic inorganic fluorides. The program is directed toward the preparation of high-purity crystals of BeF_2 in a single polymorphic form for needed thermodynamic and related properties in the ARPA's light element project at the NBS.

A special cell equipped for thermal analysis has been fabricated for the preparation of relatively large amounts (25 to 40g) of the pure crystalline forms of the individual polymorphs of BeF_2. The cell is designed for operation with solid fluorides to temperatures to 1000°C with accompanying thermal analysis. It is provided with removable containers at the bottom, lower-center, and top of the cell in which the products as solids can be removed after phase separations involving distillation, crystallization, sublimation, and preferential decomposition. These operations are performed in a hooded area with the cell placed in a vertical position in a three-zone control furnace whose temperatures are automatically controlled and recorded by remote electronic controls. Access to the cell is through a high-vacuum coupling at the top which contains an opening for evacuation and pressure control.

Cell Fabrication

A cross-section drawing of the thermal analysis and phase purification cell is shown in figure 1. It is fabricated from Inconel, nickel and Monel metal to withstand chemical attack at high temperatures both in its inner system from fluorides and in its outer system from oxidation. Inconel has excellent resistance to oxidation at high temperatures whereas nickel and Monel do not. Inconel, therefore, is used for the portion of the cell that would come in contact with atmospheric oxygen at these high temperatures. Since Inconel is not very resistant to chemical attack by fluorides, nickel is used for the inside portion of the cell that is exposed to fluorides at the high temperatures. Monel at lower temperatures resists both oxidation and chemical attacks by fluorides and is used for the high vacuum coupling, D and E in figure 1.

The machining of the various parts was designed for optimum heli-arc weld conditions to obtain non-corrosive and vacuum-tight joints in the welds between Monel and Inconel (a and e), Monel and nickel (b, c, and d) as well as the welds of the same metal (f, g, and h). The type of welds were such that no creavices were left in the inner system which is exposed to the fluorides used for the purifications and preparations. It will be noted in the figure that only two welds occur in the high temperature portion of the cell namely a weld of Inconel to Inconel at h and a butt weld of nickel to nickel at g which was designed especially to leave no creavice. All of the welds were high-vacuum tight in tests with a helium leak detector.

The cavity portion of the cell containing the removable nickel vessel 6 and its corresponding nickel and Inconel parts, in which it fits, were fabricated using an "Elox" machine with electrolytic corrosion in conjunction with machining. The straight double-wall portion (part 7 in figure) remaining after disassembly of the cell was fabricated using Inconel and nickel tubing that required little machining. Major machining was involved in the Monel coupling at the top and the cavity portions of the cell at the bottom. In addition to chemical inertness, wall thicknesses were selected for mechanical strength. Thermal expansion was provided for by a space between the double walls of Inconel and nickel comprising parts 1 and 7. Evacuation and control of the pressure of this space is provided for by "Cajan" high-vacuum couplings at C and F.

Cell Design

The cell is designed so that the products as solids after phase purifications can be removed from three different areas of the cell. The numbers in figure 1 refer to the parts in which the cell is disassembled.

Part 1 is used to collect solid from vapor in sublimation and preferential decomposition processes or as a liquid-reflux condenser in distillation processes. Nickel baffles, G, serve for these purposes. The re-entrant, coolant well, B, is for the removal of heat in these processes. For this purpose a solid rod of copper or a tube containing a liquid coolant can be inserted into the well. A thermocouple at H and another located in the coolant device placed in the well are used to obtain the temperatures of the condensation and the refluxing liquid. Part 1 is removed from the cell by six Monel bolts at the Monel high-vacuum coupling D of the Cajon type. This coupling contains openings for evacuation of the cell at A and evacuation of the double-wall space of the re-entrant coolant well at C.

Part 2 is constructed of nickel. It can be removed by turning both from the well at I and the nickel Dewar 3 as shown in figure 1.

Part 3 is a nickel Dewar for the collection of the liquid reflux in distillation processes. Its capacity is 25 cm^3. The inner and outer nickel walls of the Dewar are .020 and .030 inches thick respectively. To cut down on the emissivity, two cylinders of gold foil, .001 inch thick, were placed adjacent to the nickel walls comprising the space to be evacuated. The two cylinders of nickel were then welded in a Beamatron to form the Dewar type vessel. The vessel was then placed in a copper block composed of three parts that surrounded the vessel on the inside and outside. The copper block was then heated by the ion gun of the Beamatron to about 900°C in a chamber that was being evacuated to 10^{-5} mm Hg. After evacuation for one-half hour at this temperature and at a pressure of 10^{-5} mm Hg, the evacuated space of the Dewar was closed by welding a 1 mm hole at the tip portion of the Dewar. This technique was worked out in conjunction with the weld shop at the NBS. It is useful in that the entire vessel is subjected to the same pressure thus eliminating any possibility of wall collapse at the high temperature when the space between the walls of the Dewar are evacuated. In addition, the welds are done in a vacuum thus eliminating oxidation during welding.

Part 4 is a soft nickel gasket that was heat treated for softening to 1800°F. It is used to make a vacuum type seal between the Monel ultra-high vacuum coupling parts D and E. The gasket also extends over the tapered seat of part 5 in the coupling E; thus restricting vapor passage in the space between part 5 and the nickel-Inconel shell of the cell.

Part 5 is a nickel tube welded at d to a tapered Monel flange at the top. It surrounds the baffles, G, such that vapor passage is through the baffle area that is in contact with the re-entrant coolant well. Part 5 also serves as a radiation shield; in addition it creates a dead vapor space between its outer surface and the nickel-Inconel shell of the cell. This dead vapor space is desirable in vacuum distillations and sublimations where a residual gas pressure of about 10 mm of nitrogen or helium is purposely maintained. In this case, the residual gas would be trapped in this area thus restricting solid deposits from vapors in this space.

Part 6 is a nickel vessel that contains grooves (J in figure 1) for a tool by which it may be removed or inserted into the cell. It is constructed with a re-entrant well for contact with a thermocouple and a protrusion for crystal nucleation. Its capacity is 50 cm^3. This vessel is used to contain the solid that is subjected to phase separations and controlled heat treatment in the preparation of pure crystalline polymorphs. In distillation processes the vessel serves as the pot in which material is distilled and collected in the Dewar vessel 3. In sublimation or preferential decomposition processes, material is vaporized also from this vessel but the vaporized-to-solid product is collected on the baffles of part 1. In the case of the preferential decomposition, the wanted polymorph may remain in vessel 6 or be deposited on the baffles of part 1 depending upon whether the wanted polymorph is the less or the more volatile portion of the double salt being decomposed. In crystallization processes, the material is melted to a liquid in vessel 6, degassed by alternate freezing and melting in vacuum, and then crystallized from the liquid in the same vessel either under its own saturation vapor pressure or under the pressure of an added gas such as helium. For thermal analysis of these processes in vessel 6, the cell is equipped with a re-entrant well L and with a well, K, attached to the shell as shown in figure 1. Thermocouples at these two positions are used to determine the temperature of the contents in vessel 6 and the temperature of the cell at the same vertical position. The protrusion M, shown in figure 1, is used for nucleation of crystals from liquid when vessel 6 is used for controlled crystallizations. For this nucleation, a coolant probe surrounds the protrussion at M for the purpose of super cooling a small portion of the lqiuid at N while the bulk of the liquid in vessel 6 is at a much higher temperature. This technique has been applied quite successfully in prior researches at NBS for inducing crystallization with compounds having much lower melting points.

Part 7 in figure 1 is the portion of the cell that remains in the furnace when the cell is disassembled to remove the solid products after purifications. It consists of a double-wall shell of Inconel and nickel welded to a high-vacuum coupling, E, of Monel at c and e. The space, that was provided to accommodate differences in thermal expansion between the Inconel and nickel tubes in the shell, is evacuated and pressure controlled at the opening F. The cavity portions of the shell, which accommodate the removable vessel 6 and provide for crystal nucleation and temperature measurement of the contents of vessel 6, were fabricated from a single piece of Inconel and nickel and then joined to tubing by welds at g and h. The thermocouple port at K of Inconel was welded to the Inconel cavity portion of the shell.

Experimental Assembly for Toxic Materials

For safety in phase purifications up to 1000°C of highly toxic materials such as BeF_2, the experimental assembly for closed-system operation has been installed in a three-compartmental manner.

The high-temperature part of the assembly is in a high-exhaust hood which serves as a separate compartment. In it are located the furnace, the thermocouple leads for recording and controlling the temperatures of three furnace zones, an excess-temperature thermocouple lead for cutting off power to furnace, three power lines to furnace zones, the experimental vessel (phase purification and thermal analysis cell in this case) and the upper part of a vacuum manifold of Monel containing a nickel-Monel trap in which by-products that are solids at room temperature are collected. Descriptions and drawings of the trap, the ultra-high vacuum couplings of Monel, and the high-temperature valve of nickel and Monel, which are used in the manifold, have been reported [1]. The cell shown in figure 1 is joined at A through a Cajon ultra-high vacuum coupling of Monel to the manifold; evacuation, trapping of products removed, and pressure control of the cell during experiments is accomplished using the manifold system.

Another compartment is the cabinet under the hood, in which are located the lower-part of the vacuum manifold of Monel, a nickel-Monel trap for liquid and gases, a Monel cylinder for transfer and removal of the trapped liquid and gas, an absorption tube of Monel (for HF vapors with fluorides) and an oil mechanical pump. This cabinet has louvers on the doors, forced ventilation by a small blower into a pipe opening near the exhaust outlet of the hood, and a discharge pipe for the exhaust from the mechanical pump into this same exhaust area of the hood.

A bench area at room temperature, adjacent to the hood, is the third compartmental area on which are located the mercury diffision pump of glass and the accessories (glass traps and McLeod vacuum gage) for the high-vacuum system proper.

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[1] Augustus R. Glasgow, Jr., "Apparatus Developments for Purifications and Analyses (Thermal) to 1000°C". Chapter 8 in NBS Report No. 8186, Jan. 1, 1964, Preliminary Report on the Thermodynamic Properties of Selected Light-Element and Some Related Compounds.

The above compartmental arrangement of the experimental assembly has the following advantages. The separation of the most hazardous, high-temperature part of the apparatus from the others minimizes danger in that only a few operations at most or none at all are required in this area during an experiment. Whereas in the cabinet area, frequent attention is required in the refrigeration with liquid nitrogen of the trap for liquid and gas and in the transfer of the trap contents to a cylinder. Also in the case of a failure in the experimental vessel at the high temperature, the vacuum manifold in the hood can be isolated from the vacuum system by closing a valve in the cabinet area. The location in another area of the glass system that was available for producing and measuring a high vacuum, facilitates the much more frequent attention to this part of the system. Further, it separates the glass parts containing mercury in the diffusion pump and in the McCleod gage from the all metal system within the hood and cabinet areas, thus minimizing breakage and enhancing safety.

In setting-up a laboratory for high-temperature research with toxic materials, alterations were made in an existing hood to achieve the above separations of the apparatus assembly into three areas. However, commercially available hoods designed on this principal would appear to be of a great advantage to other workers performing experiments with toxic materials at high-temperatures under high-vacuum and controlled pressure conditions.

Furnace and Temperature Control

A three-zone furnace and a panel cabinet with instrumentation for automatically controlling and recording temperatures as e m f of three furnace zones was custom fabricated by the Hevi-Duty Electric Company according to our specifications.

The furnace is of the split-tube type with hinges and a special closing fixture and guide to permit vertical or horizontal operation. The diameter of the shell is 12 3/4 inches. The overall length is 15 1/2 inches with end transite cover plates, 1/2 inch thick, and end vestibules, 1 1/4 inches in length. A type 330 stainless stell liner (2.47 in., i.d. and 2.86 in., o.d.) 14 1/4 inches long fits into the heat chamber. It is held concentric to the heat chamber by the end vestibules and is easily removed. The heat chamber is 12 inches in length and 3 3/4 inches in diameter. It is divided into three electrically heated zones of 4 inches each, which are independently heated with separate power lines to each section. Six chromel-alumel thermocouples are located in the heating elements of the furnace chamber; one in each end zone and four in the center zone. Five of these are used for temperature control and recording. The sixth is used for the over-temperature protection instrument that automatically cuts off power to these zones if the temperature exceeds a predetermined set value.

Thermocouple lead wires from the panel cabinet in a rubber-covered cable terminate in a junction box located outside the hood. The six thermocouple leads from the furnace are connected to this box. The electric power cords to each of the three furnace zones are connected to separate power outlets that are located outside the hooded area. The current to these outlets is controlled from the panel cabinet by the e m f of the thermocouple in the furnace zone.

Three Leeds and Northrup AZAR recorders are used to control and record temperatures as e m f for the three furnace zones. The electronic assembly in the panel in addition to the AZAR recorders includes three "L and N" control units, three magnetic amplifiers and self-saturating reactors, one control circuit transformer, one constant voltage transformer, one oven-temperature protection instrument, and one main cut-off contactor.

The arrangement of the three thermocouples in the center zone for the temperature control system allows the end zones to be operated as slave systems to a master center zone. Temperature control with this system was such that the band width on the strip chart of the AZAR recorder for the center zone was constant to within several hundredths of a degree in the range of 500 to 1000°C when the end zones were operated as slaves to the center zone.

Controlled Atmosphere Dry Box

A controlled atmosphere dry box with a glove panel and accessories for maintaining a dry inert atmosphere is used in experimentation with hygroscopic substances, such as BeF_2. The controlled atmosphere is used in processes involving the filling and removal of material into or from the experimental vessel.

The glove box is basically a Kewaunee Model 2C-380R box with the exception that, in addition to the interchange compartment on one end, there is also a swinging door panel on the other end. This latter door is 14 by 14 inches and is used for inserting experimental vessels such as the phase purification and thermal analysis cell or its parts, when the material must be protected from atmospheric moisture and gases.

Figure 1

Phase Purification and Thermal Analysis Cell

1 - 7; Disassembly parts:

1 - Unit containing vapor condensor for liquid reflux or solid deposit

2 - Removable nickel support for Dewar

3 - Nickel Dewar

4 - Soft nickel gasket

5 - Nickel tube with tapered Monel flange at top

6 - Removable nickel vessel

7 - Inconel-nickel shell welded to Monel high-vacuum coupling and cavity portion for vessel 6

a - h; Welds: a, e - Monel to Inconel; f, g - Nickel to nickel
b, c, d - Monel to nickel; h - Inconel to Inconel

A - Monel, "Cajon gland", ultra-high vacuum coupling for attachment to manifold

B - Re-entrant cooling well

C, F - Monel, "Cajon body", ultra high-vacuum coupling for pressure control of space between nickel-Inconel walls

D - Monel, "Cajon-type gland", ultra-high vacuum coupling for cell

E - Monel, "Cajon-type body", ultra-high vacuum coupling for cell

G - Nickel baffles

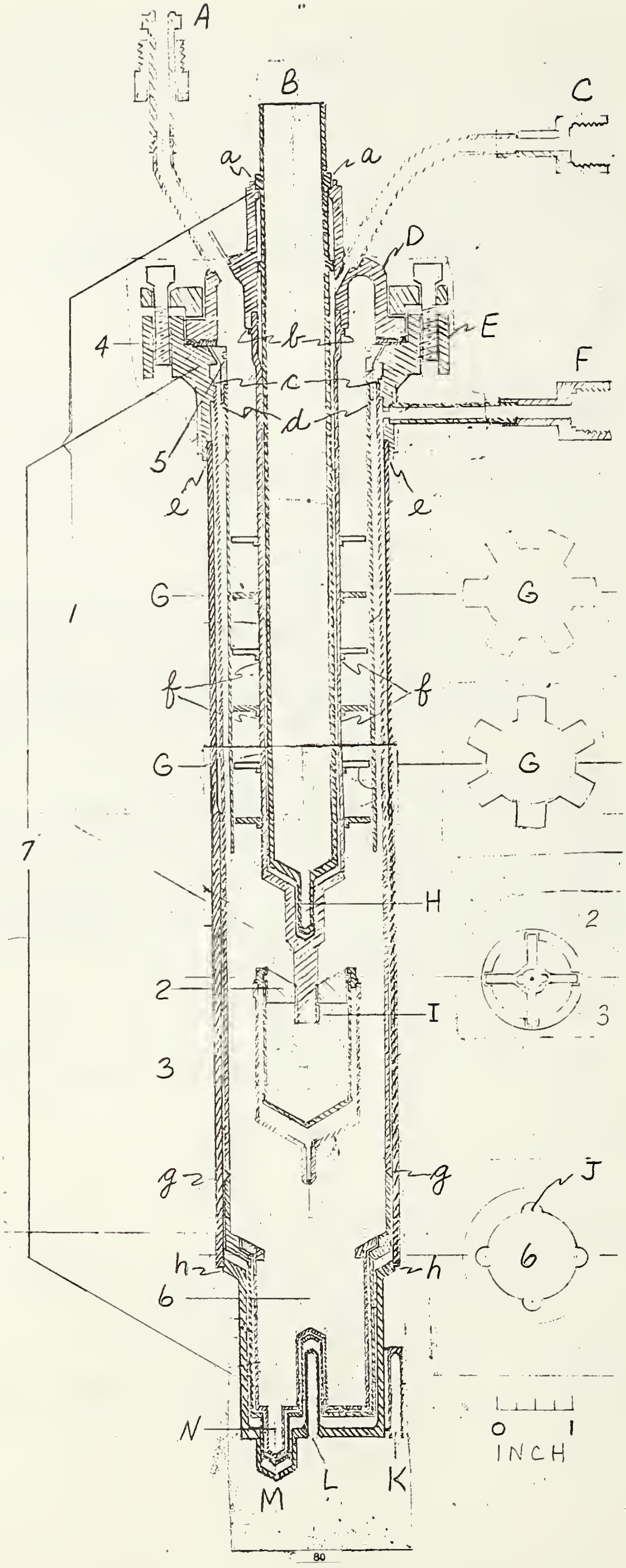
H, K, L - Thermocouple port

I - Knob used as lock-device for part 2

J - Grooves for cell-insertion or-removal tool for vessel 6

M - Protrusion for crystal nucleation in vessel 6

N - Small portion of contents of vessel 6 super cooled for crystal nucleation


A
B
C
a
a
D
E
4
b
c
F
d
5
e
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G
G
1
f
f
G
G
7
H
2
2
I
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3
g
g
J
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h
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6
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INCH

Chapter B-6

HIGH-TEMPERATURE STUDIES WITH THE ARC-IMAGE FURNACE

by J. J. Diamond and A. L. Dragoo

Rate of Vaporization of Liquid Alumina in Inert Gases.

Estimates of the rates of vaporization of liquid alumina in He, Ne and Ar, from 0.15 to 1 atm, were made using the equation (9) derived in NBS Report No. 8186. The estimated rate in 1 atm of Ar was much lower than the observed average rate of weight loss (0.31 ± 0.04 $\mu g\ cm^{-2} sec^{-1}$) given in the above mentioned report. This lack of agreement indicated that either the gas slowly flowing through the vaporization chamber was causing significant transpiration or the equation did not include all important parameters, namely convection and condensation.

Since the vaporization chamber had a large temperature gradient between the liquid alumina at the center and the walls of the flask, a transpiration experiment was impossible and the system was therefore modified to carry our vaporization measurements in 1 atm of a non-flowing gas. The results obtained in 1 atm of Ar gave an average weight loss of 0.04 ± 0.03 $\mu g\ cm^{-2} sec^{-1}$. This value is about one-tenth of the previously reported result indicating that transpiration had been significant in the earlier experiment. The large standard deviation (±0.03) was primatily due to a very small weight loss -- on the order of 20 to 30 μg -- and a significant uncertainty in weighing of the same order of magnitude -- about ± 10 μg. This uncertainty in weighing appears to depend in part on the absorption and loss of water vapor from the surface of the sample due to humidity changes in the balance room.

To obtain higher weight losses and thus to improve precision, we decided to carry out the measurements at pressures of less than 1 atm. The system was modified so that the gas can be admitted into the system through a drying tube containing P_2O_5. The system can be evacuated up to the drying tube prior to filling. The pressure of the gas in the system can be measured with a Wallace and Tiernan precision mercurial manometer, type FA-135.

The result obtained for vaporization of liquid Al_2O_3 in 1 atm of nonflowing Ar was still higher than the estimated rate indicating the process could not be described merely as diffusion of the vaporizing molecules through a surrounding gas "film." However, Elenbaas [1] has shown for the rate of evaporation of an incandescent tungsten filament in a gaseous atmosphere, that the rate of evaporation multiplied by the pressure is proportional to the dissipated heat. Turkdogan [2] has recently published a theoretical treatment of the enhancement of diffusion limited rates of vaporization by a convection-condensation process, and Turkdogan and Mills [3] have applied this theory to the vaporization of Fe-Ni alloys. Application of the theoretical treatments of Elenbaas and of Turkdogan to the vaporization of liquid Al_2O_3 in the presence of a gas is now under consideration.

Temperature Measurement

The actual temperature of molten alumina prepared with an arc-image furnace had not been conclusively determined previously nor had the major portion of the sample--liquid, interface or solid--responsible for radiation absorption been determined. Diamond and Schneider [4] reported a melting point temperature of 2025°C observed on a very small drop melted on the end of an alumina rod by means of a solar furnace. But, this would be the temperature of a much larger drop only if the interface or the solid were the major heat receptor, or if there were thermal equilibrium between the solid and liquid phases.

We measured the apparent temperature of liquid alumina in vacuum, in air and in Ar with an L & N manual optical pyrometer. The samples consisted of polycrystalline rods and tubes, varying in size from 1.0 to 9.5 mm diameter, and one 1/8 inch single-crystal sapphire rod. The observed temperature was corrected for the window of the flask (when used), the rotating shutter and the prism through which the pyrometer was sighted.

The results obtained in vacuum and in air (the temperature of 1/4 inch rod in Ar agreed closely with that in air) have been plotted as apparent temperature versus drop thickness in Figure 1. Only one point is below the approximate melting point temperature of 2050°C. The apparent temperature of liquid alumina in air has not been corrected for the spectral emissivity (which is unknown) so that it must be less than or equal to the actual temperature. Consequently, the temperature of the liquid is above the melting point temperature.

The higher apparent temperature values obtained in vacuo were due to either cooling of the liquid surface by convection of the air or a reflection contribution by the flask to the apparent temperature in vacuo. The latter possibility is being investigated at this time.

The fact that tubes and rods with drops of the same thickness had the same temperature confirmed what was demonstrated earlier with the L & N automatic optical pyrometer, that the temperature observed was that of the liquid and not the liquid-solid interface. Thus, the transmissivity of the liquid in the visible region is very low.

Since the apparent temperature exceeds the melting point, this suggests that most of the heating of the sample occurs in the liquid phase and that a thermal gradient occurs near the interface. This is supported by the observations made with the single-crystal sapphire rod. Due to the high transmissivity of sapphire it was impossible to melt it directly. However, when a thin collar (1/16 inch long) of polycrystalline alumina was placed on the end, the polycrystalline Al_2O_3 could be melted to form a drop on the end of the sapphire rod. Once the molten oxide was present on the tip of the rod, the rod could be advanced further into the focal point and extensive amounts of the rod melted. The temperature of a molten drop supported on the end of a sapphire rod also agrees well with measurements made on polycrystalline alumina, thus again demonstrating that the interface does not enter into the temperature measurement.

The increase in temperature with drop thickness arises from the fact that the larger drop penetrates further into the focal spot, and intercepts more of the highest flux at the center of the spot.

In summary, our observations indicate that the heating of the molten oxide occurs by means of the liquid phase, and therefore a steady-state heat transfer rather than thermal equilibrium exists between the liquid and the solid. The spectral transmissivity of the liquid is nearly zero, so that the temperature observed is that of a region near the surface of the liquid.

Initial observations on MgO

Observations were made to determine whether studies should be begun on MgO. When heated with the arc-image furnace in open air, white smoke arose profusely from the tip, but the sample did not melt. When heated in vacuum a dark brown deposit developed rapidly on the portion of the flask directly in front of the sample. Again, the sample did not melt. Finally the sample was heated in 1 atm of O_2 which suppressed the rate of vaporization markedly, but melting did not occur. Consequently, we believe that the high sublimation pressure of solid MgO would create considerable difficulty for study with arc-image technique by the rapid fogging of the flask and uncertainty in observed temperatures which would result.

Preparation of Beryllia-Alumina Compounds

Beryllia and alumina were mixed in one-to-one mole ratio and pressed into rods which were fused with the arc-image furnace. X-ray diffraction analysis showed about 95% $BeO.Al_2O_3$. A sample of $BeO.3Al_2O_3$ now is in preparation. These samples will be used for mass spectrometric investigations.

References

[1] W. Elenbaas, Philips Res. Repts., 18, 147-160 (1963).

[2] E. T. Turkdogan, Trans. Met. Soc. AIME 230 [4], 740-750 (1964).

[3] E. T. Turkdogan and K. C. Mills, Trans. Met. Soc. AIME 230 [4], 750-753 (1964).

[4] J. J. Diamond and S. J. Schneider, J. Am. Ceram. Soc., 43 [1], 1-3 (1960).

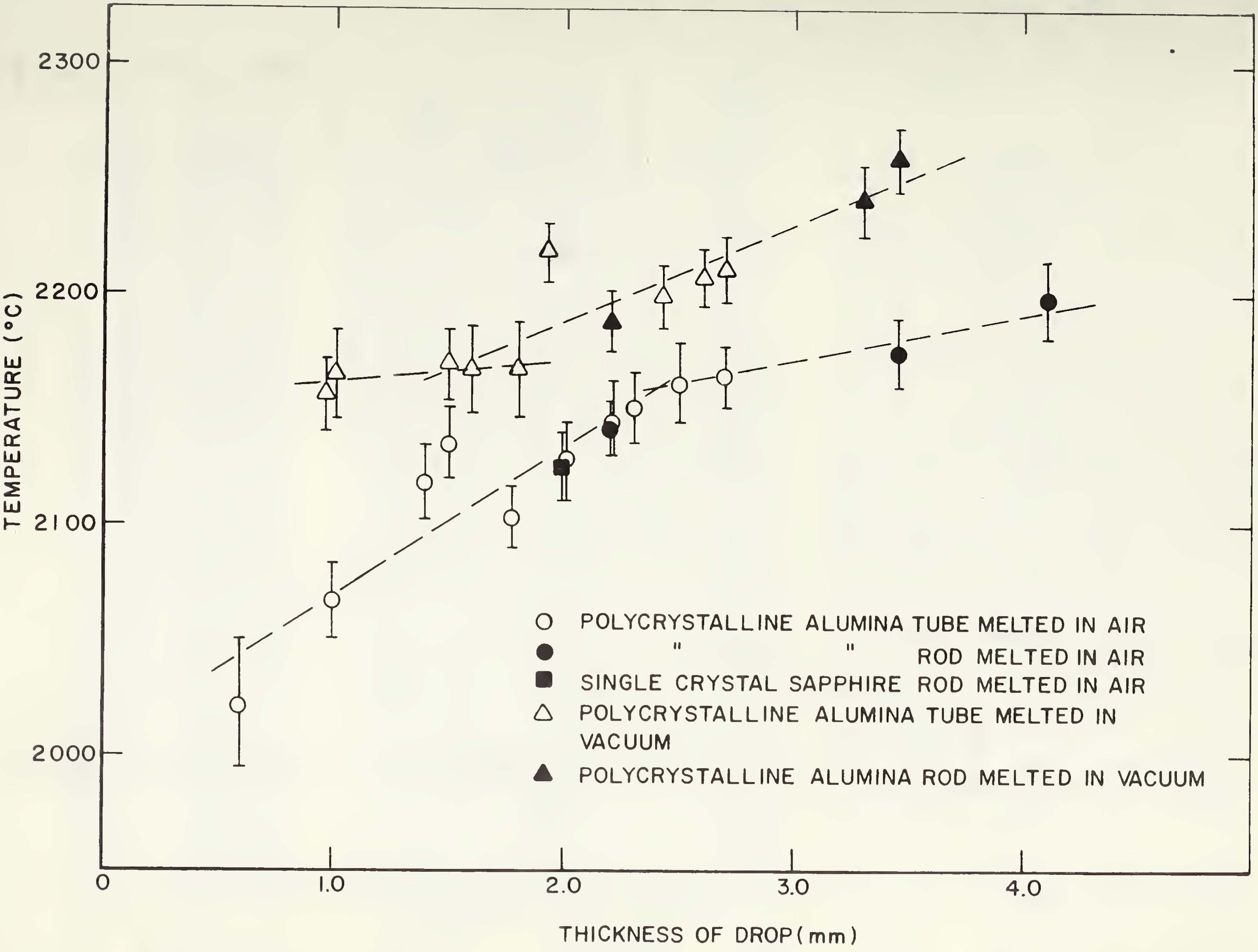

Fig. 1: Apparent temperature of liquid alumina drops melted with arc-image furnace

HIGH-TEMPERATURE MATRIX SPECTROSCOPY

D. E. Mann

For purposes of computing provisional tables of ideal-gas thermodynamic functions (see Appendix I) and applying them to the thermodynamic treatment of mass-spectrometric data (see Chapter B-8), the following estimates of molecular constants were made.

1. BeOAℓ

(a) Structure: bent; apex angle, approximately 150°

r(BeO), approximately 1.36A

r(AℓO), approximately 1.66A

Ground state: doublet (nominally, $^2\Sigma$).

(b) Vibrational spectra and multiplicities: ν_1, 1500 cm^{-1} (1)

ν_2, 1000 cm^{-1} (1)

ν_3, 275 Cm^{-1} (1)

2. BeF_2

Arguments similar to those for Li_2O and LiO lead to:

ν_1, approximately 750 cm^{-1} (1)

r(BeF), 1.34A

A. Snelson (Quarterly Technical Summary Report for Nov. 14, 1963, through Feb. 14, 1964, Report No. IITRI-C6013-3, "Optical Spectra of Some Low-Molecular-Weight Compounds Using the Matrix Isolation Technique," Illinois Institute of Technology Research Institute, Chicago, Ill.) has recently reported the following additional constants for this molecule on the assumption that it is linear:

ν_2, 320 cm^{-1} (2)

ν_3, 1535 cm^{-1} (1)

Chapter B-8

SURVEY OF HEAT CAPACITY AND HEAT CONTENT DATA OF SELECTED COMPOUNDS OF Ba, Ca, Cr, Fe, K, and Si

George T. Furukawa, William G. Saba and
Mary A. Krivanec

This report gives a survey of heat capacity and heat content data on selected compounds of Ba, Ca, Cr, Fe, K, and Si. The heat data on compounds of the above elements in combination with Aℓ, Be, O, F, Cℓ, C, and N have also been examined. The U.S. Bureau of Mines Bulletin 584 [61][1] and 592 [64] were searched initially for sources of data. The original papers and any references to other papers were examined and the experimental data compiled. The Bulletin of Thermodynamics and Thermochemistry Nos. 6 [171] and 7 [172] were surveyed for more recent publications and the data were examined wherever the original papers were immediately available. Other papers in less easily accessible publications will be examined in the future.

A survey of heat data above room temperature on most of the potassium compounds of interest has already been given in Chapter 5 of NBS Report 7192, 1 July 1961, by T. B. Douglas and W. R. Thurber. Literature surveys and calculations of thermodynamic functions of some of the potassium compounds from heat data below room temperature have been given by G. T. Furukawa and M. L. Reilly in NBS Reports 7796, 8033 and 8186. The present survey includes information on a few of the more complex potassium compounds.

The present survey lists the chemical formulas of the substances and the temperature ranges of the heat capacity (C) and relative enthalpy (ΔH) data that are available. The crystalline form of the substance is given along with the transition and melting temperatures observed or estimated by the various invesigators. The entropy at 298.16° or 298.15°K (S_{298}) is also given whenever the investigator computed the quantity from the heat-capacity data.

The symbols C and ℓ represent crystalline and liquid states of the substances, respectively. The Greek letter symbols indicate the assignments given by the authors for different crystalline forms that they had investigated.

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[1] The numbers in brackets indicate the literature references at the end of this chapter.

Reported Investigations of Heat Capacities and Heat Contents of Selected Substances

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
Ba									
	c	1907		88 - 293	100				
	c	1913		20 - 80	27				
	c	1935						(16.0 ± 0.5)	62
	c	1957				1.5 - 20	123		
	c	1961						16.0 ± 0.5	64
$BaCl_2$									
	c	1908		290 - 319	129				
	c	1909		273 - 291	130				
BaF_2									
	c	1938				14 - 301	120	23.03 ± 0.1	120
	c	1961						23.03 ± 0.10	64
BaO									
	c	1935				56 - 299	2	16.8 ± 0.3	2
	c	1951		298 - 1299	79				
	c	1961						16.8 ± 0.3	64
Ca									
	c	1907		88 - 293	100				
	c	1913		20 - 80	27				
	c	1916				22 - 62	46		
	c	1918				68 - 294	31		
	c, α, β	1924		293 - 873	32				
	α--β	1924	673		32				
	c, l	1928		293 - 1203	169				
	α--β	1928	1058		169				
	c	1930				10 - 201	18		
	c	1936				713 - 803	132		
	c	1957				1.5 - 20	123		
	α--β	1960	713		61				
	β--l	1960	1123		61				
	c	1961						9.95 ± 0.10	64

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
CaC_2									
	c	1941				53 - 295	57	16.8 ± 0.5	57
	c	1943		298 - 1271	91				
	c	1961						16.8 ± 0.4	64
$CaCl_2$									
	c	1913		289 - 823	85				
	c	1943				53 - 295	65	27.2 ± 0.4	65
	c	1943		298 - 1667	90				
	c	1961						27.2 ± 0.3	64
CaF_2									
	c	1911		83 - 273	74				
	c	1913				18 - 86	38		
	c	1935		288 - 1273	77				
	c, l	1945		298 - 1800	97				
	α--β	1945	1424		97				
	β--l	1945	1691		97				
	c	1949				54 - 296	145	16.46 ± 0.08	145
	c	1961						16.46 ± 0.08	64
CaO									
	c	1908		293 - 953	81				
	c	1911				83 - 273	74		
	c	1913		289 - 1037	85				
	c	1914				28 - 89	99		
	c	1919		293 - 2825	158				
	c	1926				87 - 293	110	9.6	110
	c	1929		293 - 1125	125				
	c	1930		289 - 577	73				
	c	1933		273 - 1773	34				
	c	1933		273 - 1473	35				
	c	1935		293 - 1183	82				
	c	1951		298 - 1176	79				
	c	1961						9.5 ± 0.2	64

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
$CaO.Al_2O_3$	c	1933		293 - 1673	34				
	c	1955				54 - 296	69	27.3 ± 0.2	69
	c	1955		298 - 1800	11				
	c	1961						27.3 ± 0.2	64
$CaO.2Al_2O_3$	c	1955				54 - 296	69	42.5 ± 0.3	69
	c	1955		298 - 1802	11				
	c	1961						42.5 ± 0.3	64
$3CaO.Al_2O_3$	c	1933		293 - 1573	34				
	c	1955				54 - 297	69	49.1 ± 0.3	69
	c	1955		298 - 1808	11				
	c	1961						49.1 ± 0.3	64
$12CaO.7Al_2O_3$	c	1955				54 - 297	69	249.7 ± 1.5	69
	c	1955		298 - 1673	11				
	α--β	1955	1310		11				
	c	1961						249.7 ± 1.5	64
$CaO.Al_2O_3.2SiO_2$ (anorthite)	c	1919		273 - 1673	164				
	c	1957				53 - 296	71	48.4 ± 0.4	71
	c	1961						48.4 ± 0.3	64
$CaO.Al_2O_3.2SiO_2$	gl	1919		273 - 973	164				
$2CaO.Al_2O_3.SiO_2$ (gehlenite)	c	1933		293 - 1573	34				
$CaO.Fe_2O_3$	c	1954				53 - 296	68	34.7 ± 0.2	68
	c	1954		298 - 1805	10				
	c	1961						34.7 ± 0.2	64

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
$2CaO.Fe_2O_3$	c	1954				53 - 296	68	45.1 ± 0.3	68
	c	1954		298 - 1838	10				
	c	1961						45.1 ± 0.3	64
$CaO.SiO_2$ (wollastonite)	c, β	1909		298 - 1373	162				
	c, β	1919		273 - 1573	164				
	c, β	1929		293 - 1157	125				
	c, β	1932		290 - 1369	157	10 - 304	157		
	c, β	1933		293 - 1773	34				
	c, β	1934				10 - 210	22		
	c, β	1941		298 - 1423	140				
	c, β	1961						19.6 ± 0.2	64
$CaO.SiO_2$ (pseudo-wollastonite)	c, α	1909		298 - 1573	163				
	c, α	1909		298 - 1573	162				
	c, α	1919		273 - 1673	164				
	β--α	1919	1443		164				
	c, α	1926				88 - 298	111		
	c, α	1932		291 - 1558	157	11 - 295	157		
	c, α	1961						20.9 ± 0.2	64
$CaO.SiO_2$	gl	1919		273 - 973	164				
$2CaO.SiO_2$	c	1933		293 - 1573	34				
	γ--β	1933	948		34				
	c, β	1951				53 - 296	146	30.5 ± 0.2	146
	c, γ	1957				54 - 296	71	28.8 ± 0.2	71

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
$2CaO.SiO_2$									
	c, α, α', β, γ	1957		298 - 1816	21				
	γ--α'	1957	1120		21				
	α'--α	1957	1710		21				
	β--α'	1957	970 (metastable)		21				
	c, β	1961						30.5 ± 0.2	64
	c, γ	1961						28.8 ± 0.2	64
$3CaO.SiO_2$									
	c	1933		293 - 1773	34				
	c	1951				54 - 297	146	40.3 ± 0.3	146
	c	1961						40.3 ± 0.3	64
$3CaO.2SiO_2$									
	c	1957				53 - 296	71	50.4 ± 0.3	71
	c	1961						50.4 ± 0.3	64
Cr									
	c	1913		20 - 80	27				
	c	1914		291 - 867	131				
	c	1918		273 - 2773	168				
	c	1926		289 - 1913	153				
	c	1927				71 - 79	138		
	c	1934		293 - 1339	52				
	c	1937				56 - 291	4	5.68 ± 0.05	4
	c	1950				273 - 1073	6		
	α--β	1952	2113		9				
	β--l	1952	2176		9				
	c	1952				1.8 - 4.2	37		
	c	1955				1.2 - 20	167		
	c	1956				1.5 - 4.2	122		
	c	1958				964 - 1595	76		

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
Cr	c	1961						5.68 ± 0.07	64
	c	1962				14 - 274	17	5.64 ± 0.03	17
$CrCl_2$	c	1937				44 - 296	4	27.4 ± 0.7	4
	c	1961						27.7 ± 0.7	64
	c	1962				11 - 299	142	27.56 ± 0.05	142
$CrCl_3$	c	1936				12 - 129	150		
	c	1936				12 - 129	151		
	c	1937				54 - 297	4	28.2 ± 1.0	4
	c	1958				12 - 308	47	29.38	47
	c	1961						29.4 ± 0.2	64
CrF_3	c	1958				15 - 308	47	22.438	47
	c	1961						22.44 ± 0.10	64
Cr_2O_3	c	1912		82 - 323	126				
	c	1935		288 - 1428	82				
	c	1937				56 - 336	4	19.4 ± 0.2	4
	c	1944		298 - 1774	63				
	c	1961						19.4 ± 0.3	64
Cr_3C_2	c	1944		298 - 1576	63	53 - 295	63	20.4 ± 0.2	63
	c	1953				13 - 301	26	20.42 ± 0.5	26
	c	1954		273 - 1188	107				
	c	1961						20.42 ± 0.10	64
Cr_5C_2	c	1944				55 - 295	63	(33.9 ± 0.3)	63
Cr_7C_3	c	1944		298 - 1578	63	54 - 295	63	48.00 ± 0.3	63
	c	1961						48.0 ± 0.3	64

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
$Cr_{23}C_6$									
	c	1944		298 - 1695	63	55 - 295	63		
	c	1961						145.8 ± 0.7	64
Fe									
	c	1873		282 - 1173	160				
	c	1886		273 - 1279	116				
	c	1886		273 - 1473	117				
	c	1888		288 - 585	94				
	c	1905		293 - 923	143				
	c	1905		273 - 1417	48				
	c	1907		273 - 1796	101				
	c	1907		88 - 293	100				
	c	1912				383 - 1241	119		
	c	1913		290 - 953	83				
	c	1913		20 - 80	27				
	c	1914				50 - 390	44		
	c	1914		291 - 903	131				
	c	1916				32 - 95	46		
	c	1917				737 - 1203	161		
	c, l α, β, γ, Δ	1918		273 - 1873	168				
	α--β	1918	1033		168				
	β--γ	1918	1183		168				
	γ--Δ	1918	1673		168				
	Δ--l	1918	1812		168				
	c	1925				73 - 198	124		
	c	1926		303 - 523	54				
	c, l	1926		293 - 1903	153				
	c--l	1926	1793		153				
	c, l	1927		273 - 1863	102				
	c--l	1927	1801		102				
	c	1927		291 - 1233	154				

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
Fe	c	1927				373 - 1273	72		
	c	1928		291 - 1173	169				
	c	1928				292 - 667	24		
	c, l	1929		289 - 1833	155				
	c	1929		293 - 1104	125				
	c	1930				17 - 206	39		
	c	1932		review	7				
	c	1935				30 - 220	139		
	c	1935		273 - 1533	87				
	c	1936				291 - 1233	80		
	c	1938				373 - 673	144		
	c	1938		298 - 1764	170				
	c	1938		298 - 1764	53				
	c	1939				1.5 - 20	29		
	c	1939				1.1 - 20.4	55		
	c	1940				323 - 1223	8		
	c	1941				293 - 1373	36		
	c	1943				55 - 295	60	6.49 ± 0.03	60
	c	1949				273 - 1523	109		
	c	1951		review	23				
	c--l	1954	1812 ± 2		106				
	α--γ	1955	1184		13				
	γ--Δ	1955	1665		13				
	Δ--l	1955	1809		13				
	curie	1955	1042		13				
	c, l	1956		303 - 1919	113				
	c, γ, Δ	1959		1193 - 1789 (relative to 298)	105				
	c	1961						6.49 ± 0.03	64

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
Fe	c, α, γ	1962		300 - 1433	5				
	c	1963				1073 - 1673	25		
	α--β	1963	1033		25				
	β--γ	1963	1187		25				
	γ--Δ	1963	1664		25				
	Δ--l	1963	1809		25				
Fe_3C	c	1934		85 - 1036 (relative to 298)	95				
	c	1939				68 - 297	133	25.7 ± 1.0	133
	c	1961						24.2 ± 1.0	64
Fe.C(4.22 percent)	c	1926		294 - 1623	153				
Fe(1-x).C(x) (x = 0.06 to 4.03 percent, 7 specimens)	c	1908		273 - 923	103				
(x = 0.11 to 4.06 percent, 20 specimens)	c	1913		290 - 953	83				
(x = 0.09 to 2.84 percent, 12 specimens)	c	1926		293 - 1523	152				
(x = 0.04 to 0.770 percent, 5 specimens)	c	1927		291 - 1243	154				
(x = 0.07 to 5.07 percent, 19 specimens)	c	1935		288 - 1843	156				
(x = 0.075 to 3.36 percent, 13 specimens)	c	1941				293 - 1313	36		
$FeCl_2$	c	1936		288 - 913	78				
	c	1936				16 - 127	149		
	c	1936				16 - 127	151		
	c	1943				53 - 295	65	28.7 ± 0.8	65
	c	1943		298 - 1080	90				
	c	1961						28.7 ± 0.5	64

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
$FeCl_3$	c	1951		298 - 561	148	53 - 297	148	32.2 ± 0.4	148
	c	1961						32.2 ± 0.4	64
FeF_2	c	1955				11 - 307	16	20.79 ± 0.04	16
	c	1961						20.79 ± 0.06	64
$Fe(0.947)O$	c	1951				54 - 296	147	14.2 ± 0.2	147
	c, l	1951		298 - 1784	20				
	c--l	1951	1650		20				
	c	1952						13.74 ± 0.10	49
	c	1961						13.74 ± 0.10	64
FeO	c	1929				71 - 302	89	12.7 ± 2.0	89
	c	1933		303 - 1173	165				
$FeO.Al_2O_3$	c	1932		323 - 1298	112				
	c	1956				53 - 296	70	25.4 ± 0.2	70
	c	1961						25.4 ± 0.2	64
$FeO.Cr_2O_3$	c	1932		323 - 1298	112				
	c	1944		298 - 1787	96				
	c	1944				53 - 296	135	34.9 ± 0.4	135
	c	1961						34.9 ± 0.4	64
$2FeO.SiO_2$	c	1929		293 - 1161	125				
	c	1933		273 - 1473	35				
	c	1941				52 - 295	59	35.4 ± 1.4	59
	c	1953		298 - 1724	108				
	c	1961						34.7 ± 0.4	64

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. ^{o}K	Relative Enthalpy Range ^{o}K	Ref.	Heat Capacity Range ^{o}K	Ref.	S_{298} cal/deg-mole	Ref.
Fe_2O_3									
	c	1912		81 - 317	126				
	c	1926				273 - 923	15		
	c, α	1926				88 - 289	110	21.5	110
	c	1929		293 - 1097	125				
	c	1930		291 - 630	73				
	c	1951		298 - 1757	20				
	α--β	1951	950		20				
	β--γ	1951	1050		20				
	c, α	1959				6 - 345	45	20.889	45
	c, α	1961						20.90 ± 0.10	64
Fe_3O_4									
	c	1917				296 - 954	161		
	c	1926				90 - 295	110	35.1	110
	c	1929				60 - 300	89	34.69 ± 0.2	89
	c	1929		293 - 1056	125				
	c	1932		323 - 1298	112				
	c	1933		273 - 1273	35				
	c, α, β	1951		298 - 1825	20				
	α--β	1951	900		20				
	c	1956				1.8 - 4.2	75		
	c	1961						35.0 ± 0.6	64
$KAlSiO_4$ (kaliophilite)									
	c	1953				53 - 296	67	31.8 ± 0.3	67
	c	1961						31.8 ± 0.3	64
$KAlSi_2O_6$ (leucite)									
	c	1953				53 - 296	67	44.0 ± 0.4	67
	c	1961						44.0 ± 0.4	64
$KAlSi_3O_8$ (orthoclase)									
	c	1909		273 - 1373	162				

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
$KAlSi_3O_8$	gl	1909		273 - 1373	162				
	gl	1919		273 - 1373	164				
$KAlSi_3O_8$ (microcline)	c	1919		273 - 1173	164				
$KAlSi_3O_8$ (adularia)	c	1953				54 - 297	67	52.5 ± 0.5	67
	c	1961						52.5 ± 0.5	64
$KAlSi_3O_8$ (ferriferous orthoclase)	c	1953				54 - 296	67		
K_2CrO_4	c	1956				60 - 300	121	47.8 ± 0.8	121
	c	1961						47.8 ± 0.8	64
$K_2Cr_2O_7$	c	1909		298 - 757	43				
	c	1956				80 - 300	121	69.6 ± 1.7	121
	c	1961						69.6 ± 1.7	64
Si	c	1907		88 - 293	100				
	c	1912		82 - 319	126				
	c	1913		20 - 80	27				
	c	1914				20 - 90	99		
	c	1923		290 - 1174	86				
	c	1930				61 - 296	1		
	c	1952				1 - 100	114		
	c	1952		273 - 1509	134				
	c	1957		1473 - 1823	104				
	c	1959				7.7 - 300	41	4.497 ± 0.009	41
	c	1961						4.51 ± 0.05	64
Si (amorphous)	c	1912		83 - 325	126				

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
SiC	c	1912		84 - 316	126				
	c	1914				22 - 96	99		
	c	1915		273 - 1224	159				
	c	1916				25 - 75	46		
	c	1923		290 - 1173	86				
	c	1926		290 - 1676	88				
	c	1941				54 - 295	58		
	c (hex)	1952		298 - 1789	50	54 - 296	50	3.94 ± 0.02	50
	c (cubic)	1952		298 - 1693	50	54 - 296	50	3.97 ± 0.02	50
	c (hex)	1961						3.94 ± 0.02	64
	c (cubic)	1961						3.97 ± 0.02	64
SiO_2 (quartz)	c	1888		273 - 1458	118				
	c	1909		273 - 1373	162				
	c	1911				26 - 93	98		
	c	1911		79 - 273	74				
	c	1913		289 - 825	85				
	c	1915		273 - 1973	166				
	c	1918		273 - 1773	168				
	c	1919		273 - 1373	164				
	c	1920		273 - 1673	12				
	c	1923				701 - 925	115		
	c	1924		293 - 1273	19				
	c	1926		288 - 1898	88				
	c	1929		293 - 1171	125				
	c	1930		291 - 623	73				
	c	1933		273 - 1373	35				
	c	1935		273 - 1473	87				
	c	1936				53 - 296	3	10.06 ± 0.1	3
	c	1936		317 - 949	92				

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
SiO_2 (quartz)									
	c	1941		298 - 554	93				
	c	1951		273 - 717	141				
	c	1961						10.00 ± 0.10	64
SiO_2 (cristobalite)									
	c	1915		273 - 1973	166				
	c	1919		273 - 1673	164				
	c	1922				29 - 117	136		
	c	1924		293 - 1273	19				
	c	1936				55 - 297	3	10.34 ± 0.1	3
	c	1941		298 - 622	93				
	c	1961						10.20 ± 0.10	64
SiO_2 (tridymite)									
	c	1936				54 - 295	3	10.50 ± 0.2	3
	c	1941		298 - 625	93				
	c	1961						10.4 ± 0.2	64
SiO_2 (amorphous)									
	c	1911		79 - 273	74				
	c	1913		287 - 824	85				
	c	1924		293 - 1273	19				
SiO_2 (coesite)									
	c	1956						8.6 ± 0.7	84
SiO_2	gl	1911				26 - 84	98		
	gl	1915		273 - 1973	166				
	gl	1919		273 - 1173	164				
	gl	1919		293 - 1039	51				
	gl	1920		291 - 1137	14				
	gl	1922				19 - 288	136		
	gl	1924		273 - 1319	128				

Chemical Formula	Physical State	Year of Report	Trans. or Melt. Temp. °K	Relative Enthalpy Range °K	Ref.	Heat Capacity Range °K	Ref.	S_{298} cal/deg-mole	Ref.
SiO_2	gl	1926				10 - 13	137		
	gl	1926		290 - 1743	88				
	gl	1929		293 - 1127	125				
	gl	1931		91 - 577	40				
	gl	1936		324 - 936	92				
	gl	1941		298 - 1795	140				
	gl	1946		298 - 1500	66				
	gl	1950		298 - 1470	33				
	gl	1959				2.3 - 19	42		
	gl	1961						S(298)-S(0)= 10.35 ± 0.10	64
								S(0)=0.9 ± 0.3	64
Si_3N_4	c	1938		273 - 858	127				
	c	1938						(22.8)	56

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Chapter B-9

MASS SPECTROMETRIC STUDY OF THE $BeO-Al_2O_3$ and BeF_2 SYSTEMS

by J. Efimenko

I. The $BeO-Al_2O_3$ System

This is a preliminary report of the mass spectrometric study of the vapor species in equilibrium over selected compositions of the Al_2O_3-BeO system.

It was reported by Lang, Fillmore and Maxwell (J. Res. NBS. 48, 301 (1952)) that the beryllia-alumina phase diagram has three eutectics and two compounds.

Eutectic Composition	Melting Point
1 BeO: 4 Al_2O_3 (94.2 wgt %)	1890°±10°C
2 BeO: 3 Al_2O_3 (85.9 wgt %)	1850°±10°C
BeO: Al_2O_3 (75 wgt %)	1835°±10°C

Compounds	Melting Point
$BeO\cdot 3Al_2O_3$	1910°±10°C
$BeO\cdot Al_2O_3$	1870°±10°C

The vaporization from these well-defined compositions will be studied.

Experimental

A specimen of prepared $BeO\cdot Al_2O_3$ was volatilized in a W effusion cell and the vapor species were observed mass spectrometrically. Temperature - ion intensity data for the species Be^+, Al^+ and $(BeO)_2{}^+$ indicated that this compound was partially reduced initially and did not correspond to the composition $BeO\cdot Al_2O_3$.

The 1:1 compound was synthesized from carbon-free alumina and sintered beryllia contained in a W cup inside the W effusion cell. X-ray diffraction analysis of this compound indicated the $BeO-Al_2O_3$ compound pattern with a slight trace of Al_2O_3.

In the temperature range 2200-2500°K the gaseous specie, $AlOBe^+$, corresponding to m/e of 52 was observed. Analysis of the data obtained in this system indicated excessive scatter, not permitting quantitative conclusions to be formed. Repetitive experiments are in progress under more controlled conditions.

Discussion

The reactions considered for this system are the following:

$$(1)\ Al(g) + Be(g) + O(g) = AlOBe(g)$$

$$(2)\ 2Al(g) + O(g) = Al_2O(g)$$

A third reaction arises from the combination of equations (1) and (2).

$$(3)\ Be(g) + Al_2O(g) = BeOAl(g) + Al(g)$$

Preliminary calculations based on tentative free energy functions for AlOBe(g) (Table A-90 in the present report) indicate reasonable values for enthalpies of reactions for (1), (3) and (2) but the estimated errors are rather large. It appears that the enthalpy of reaction for (3) should be positive and small.

II. Revision of the Enthalpy of Reaction for the $BeO \cdot BeF_2$ System

The heat of reaction ΔH_0°, computed from the experimental data on the Be_2OF_2 specie (NBS Report 8186, Ch. 13, Jan. 1, 1964) and those computed from the free energy functions given in Table A-51 (NBS Report 6928, July 1960) indicated that an error probably existed in the bending frequencies assigned to BeF_2. Similar computations based on free energy functions obtained on basis of semi-empirical relations suggested by D. L. Hildenbrand gave ΔH_0° values that were lower than the experimental one.

D. E. Mann, Chapter B-7 of this report, selected a "best" set of frequencies and a new bond length for BeF_2 molecule: 1535 cm^{-1}, 320 cm^{-1}, 750 cm^{-1} and Be-F = 1.34Å. On the basis of these revised values, new free energy functions were computed for BeF_2, as the revised Table A-51 in the present report. With the aid of this revised table and the free energy functions for BeO and Be_2OF_2, corrected ΔH_0° values for Be_2OF_2 were obtained, giving a mean ΔH_0° = 42.6 Kcal/mol for the entire set of experimental points. A comparison of the experimentally based ΔH_0° values and those based on the revised free energy functions are shown in Table 1. From this table it is evident that ΔH_0° values based on bending frequency 825 cm^{-1} gave ΔH_0° values higher than the experimental ones while bending frequency of 240 cm^{-1} gave ΔH_0° values lower than experimental ΔH_0°. The ΔH_0° values based on the free energy functions selected show no trend with temperature.

TABLE I

Mean Enthalpies of Reaction, corrected to 0°K
$BeO(s) + BeF_2(g) = Be_2OF_2(g)$

Index No.	T°K Average	Exp. Slope	825 cm^{-1} (BeF_2) FEF	Δ
1-13	1700	39.2±3.5	46.9	+7.7
21-43	2000	41.3±0.9	49.0	+7.7
			320 cm^{-1} (BeF_2)	
1-13	1700	40.4±3.5	42.1	+1.7
21-43	2000	42.5±0.9	42.9	+0.4
			240 cm^{-1} (BeF_2)	
1-13	1700	40.7±3.5	37.9	-2.8
21-43	2000	42.7±0.9	37.5	-5.2

APPENDIX I

IDEAL–GAS THERMODYNAMIC FUNCTIONS

by

Joseph Hilsenrath and Carla G. Messina

Tables of thermodynamic functions are given for the negative ions H^-, O^-, F^-, Cl^-, and for the molecule ions N_2^+, O_2^+, and NO^+. The tables are given in units of calories, moles, and °K at 273.15°, 298.15°, and 1,000(100) 10,000° K.

The negative ions are computed for the ground state, the configuration for which was taken to be that of the isoelectronic neutral atom. Thus these tables contain the translational contribution, augmented simply by ln (2J+1), where J is the principal quantum number of the ground state of the next higher neutral atom. The new scale of atomic masses was used (J. Am. Chem. Soc. [16] 80, 4121–4124, 1958).

The following constants were used in the calculation: 0.0005486 for the rest mass of a mole of electrons, 3.664943 for the Sackur–Tetrode constant, and 1.98717 cal/mole °K for the gas constant.

The tables for N_2^+, O_2^+, NO^+ were obtained from unpublished calculations of L. Haar. These values represent improvements over earlier values published by Haar and Beckett (Proceedings of the Conference on Thermodynamic and Transport Properties of Fluids, pp 27–33, Institution of Mechanical Engineers, London, 1959.)

IDEAL-GAS THERMODYNAMIC FUNCTIONS FOR NINE DIATOMIC HYDRIDES, LiO, BeF_2, and BeOAℓ

by William H. Evans

The data used in the calculations for the diatomic hydrides were taken from Herzberg (Spectra of Diatomic Molecules, 2nd Ed., Van Nostrand, New York, 1950). They refer to the isotopic species given there, but are based on the 1961 atomic masses. The data for LiO are from White, Seshadri, Dever, Mann, and Linevsky (J. Chem. Phys. 39, 2463 (1963)).

In these calculations for the hydride molecules an upper cutoff has been applied to the summations in the rotational and vibrational partition functions. This is taken as the dissociation energy of the level. This has the effect of lowering the number of available states, especially at high temperatures, and thus lowering the thermal functions. It is felt, however, that this gives a more realistic set of functions to combine with atomic functions for equilibrium calculations.

In the calculations for BeF_2 and BeOAℓ, no upper cutoff was used. For the data used, see Chapter B-7 (p. 85).

Table A-1-N Thermodynamic Functions for H^-

T °K	$\frac{-(F^\circ - H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
273.15	20.6126	4.9679	25.5805	4.9679	1357.0
298.15	21.0477	4.9679	26.0156	4.9679	1481.2
1000.	27.0596	4.9679	32.0276	4.9679	4967.9
1100.	27.5331	4.9679	32.5010	4.9679	5464.7
1200.	27.9654	4.9679	32.9333	4.9679	5961.5
1300.	28.3630	4.9679	33.3310	4.9679	6458.3
1400.	28.7312	4.9679	33.6991	4.9679	6955.1
1500.	29.0739	4.9679	34.0419	4.9679	7451.9
1600.	29.3946	4.9679	34.3625	4.9679	7948.7
1700.	29.6957	4.9679	34.6637	4.9679	8445.5
1800.	29.9797	4.9679	34.9476	4.9679	8942.3
1900.	30.2483	4.9679	35.2162	4.9679	9439.1
2000.	30.5031	4.9679	35.4711	4.9679	9935.8
2100.	30.7455	4.9679	35.7134	4.9679	10432.6
2200.	30.9766	4.9679	35.9446	4.9679	10929.4
2300.	31.1975	4.9679	36.1654	4.9679	11426.2
2400.	31.4089	4.9679	36.3768	4.9679	11923.0
2500.	31.6117	4.9679	36.5796	4.9679	12419.8
2600.	31.8065	4.9679	36.7745	4.9679	12916.6
2700.	31.9940	4.9679	36.9620	4.9679	13413.4
2800.	32.1747	4.9679	37.1426	4.9679	13910.2
2900.	32.3490	4.9679	37.3170	4.9679	14407.0
3000.	32.5175	4.9679	37.4854	4.9679	14903.8
3100.	32.6803	4.9679	37.6483	4.9679	15400.6
3200.	32.8381	4.9679	37.8060	4.9679	15897.4
3300.	32.9909	4.9679	37.9589	4.9679	16394.2
3400.	33.1393	4.9679	38.1072	4.9679	16890.9
3500.	33.2833	4.9679	38.2512	4.9679	17387.7
3600.	33.4232	4.9679	38.3911	4.9679	17884.5
3700.	33.5593	4.9679	38.5273	4.9679	18381.3
3800.	33.6918	4.9679	38.6597	4.9679	18878.1
3900.	33.8209	4.9679	38.7888	4.9679	19374.9
4000.	33.9466	4.9679	38.9146	4.9679	19871.7
4100.	34.0693	4.9679	39.0372	4.9679	20368.5
4200.	34.1890	4.9679	39.1569	4.9679	20865.3
4300.	34.3059	4.9679	39.2738	4.9679	21362.1
4400.	34.4201	4.9679	39.3881	4.9679	21858.9
4500.	34.5318	4.9679	39.4997	4.9679	22355.7
4600.	34.6410	4.9679	39.6089	4.9679	22852.5
4700.	34.7478	4.9679	39.7157	4.9679	23349.2
4800.	34.8524	4.9679	39.8203	4.9679	23846.0
4900.	34.9548	4.9679	39.9228	4.9679	24342.8
5000.	35.0552	4.9679	40.0231	4.9679	24839.6
5100.	35.1536	4.9679	40.1215	4.9679	25336.4
5200.	35.2500	4.9679	40.2180	4.9679	25833.2
5300.	35.3447	4.9679	40.3126	4.9679	26330.0
5400.	35.4375	4.9679	40.4055	4.9679	26826.8
5500.	35.5287	4.9679	40.4966	4.9679	27323.6
5600.	35.6182	4.9679	40.5861	4.9679	27820.4
5700.	35.7061	4.9679	40.6741	4.9679	28317.2
5800.	35.7925	4.9679	40.7605	4.9679	28814.0
5900.	35.8775	4.9679	40.8454	4.9679	29310.8
6000.	35.9610	4.9679	40.9289	4.9679	29807.5

Table A-1-N Thermodynamic Functions for H^- - continued

T °K	$\frac{-(F^\circ - H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
6100.	36.0431	4.9679	41.0110	4.9679	30304.3
6200.	36.1239	4.9679	41.0918	4.9679	30801.1
6300.	36.2033	4.9679	41.1713	4.9679	31297.9
6400.	36.2816	4.9679	41.2495	4.9679	31794.7
6500.	36.3586	4.9679	41.3265	4.9679	32291.5
6600.	36.4344	4.9679	41.4024	4.9679	32788.3
6700.	36.5092	4.9679	41.4771	4.9679	33285.1
6800.	36.5828	4.9679	41.5507	4.9679	33781.9
6900.	36.6553	4.9679	41.6232	4.9679	34278.7
7000.	36.7268	4.9679	41.6947	4.9679	34775.5
7100.	36.7972	4.9679	41.7652	4.9679	35272.3
7200.	36.8667	4.9679	41.8346	4.9679	35769.1
7300.	36.9352	4.9679	41.9032	4.9679	36265.9
7400.	37.0028	4.9679	41.9708	4.9679	36762.6
7500.	37.0695	4.9679	42.0374	4.9679	37259.4
7600.	37.1353	4.9679	42.1032	4.9679	37756.2
7700.	37.2003	4.9679	42.1682	4.9679	38253.0
7800.	37.2644	4.9679	42.2323	4.9679	38749.8
7900.	37.3276	4.9679	42.2956	4.9679	39246.6
8000.	37.3901	4.9679	42.3581	4.9679	39743.4
8100.	37.4519	4.9679	42.4198	4.9679	40240.2
8200.	37.5128	4.9679	42.4807	4.9679	40737.0
8300.	37.5730	4.9679	42.5410	4.9679	41233.8
8400.	37.6325	4.9679	42.6004	4.9679	41730.6
8500.	37.6913	4.9679	42.6592	4.9679	42227.4
8600.	37.7494	4.9679	42.7173	4.9679	42724.2
8700.	37.8069	4.9679	42.7748	4.9679	43220.9
8800.	37.8636	4.9679	42.8316	4.9679	43717.7
8900.	37.9198	4.9679	42.8877	4.9679	44214.5
9000.	37.9753	4.9679	42.9432	4.9679	44711.3
9100.	38.0302	4.9679	42.9981	4.9679	45208.1
9200.	38.0845	4.9679	43.0524	4.9679	45704.9
9300.	38.1382	4.9679	43.1061	4.9679	46201.7
9400.	38.1913	4.9679	43.1592	4.9679	46698.5
9500.	38.2439	4.9679	43.2118	4.9679	47195.3
9600.	38.2959	4.9679	43.2638	4.9679	47692.1
9700.	38.3474	4.9679	43.3153	4.9679	48188.9
9800.	38.3983	4.9679	43.3663	4.9679	48685.7
9900.	38.4488	4.9679	43.4167	4.9679	49182.5
10000.	38.4987	4.9679	43.4666	4.9679	49679.2

Table A-8-N Thermodynamic Functions for O^-

T °K	$-\frac{(F^\circ - H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
273.15	31.6065	4.9679	36.5744	4.9679	1357.0
298.15	32.0416	4.9679	37.0095	4.9679	1481.2
1000.	38.0535	4.9679	43.0215	4.9679	4967.9
1100.	38.5270	4.9679	43.4950	4.9679	5464.7
1200.	38.9593	4.9679	43.9272	4.9679	5961.5
1300.	39.3570	4.9679	44.3249	4.9679	6458.3
1400.	39.7251	4.9679	44.6930	4.9679	6955.1
1500.	40.0679	4.9679	45.0358	4.9679	7451.9
1600.	40.3885	4.9679	45.3564	4.9679	7948.7
1700.	40.6897	4.9679	45.6576	4.9679	8445.5
1800.	40.9736	4.9679	45.9415	4.9679	8942.3
1900.	41.2422	4.9679	46.2102	4.9679	9439.1
2000.	41.4970	4.9679	46.4650	4.9679	9935.8
2100.	41.7394	4.9679	46.7074	4.9679	10432.6
2200.	41.9705	4.9679	46.9385	4.9679	10929.4
2300.	42.1914	4.9679	47.1593	4.9679	11426.2
2400.	42.4028	4.9679	47.3707	4.9679	11923.0
2500.	42.6056	4.9679	47.5735	4.9679	12419.8
2600.	42.8005	4.9679	47.7684	4.9679	12916.6
2700.	42.9879	4.9679	47.9559	4.9679	13413.4
2800.	43.1686	4.9679	48.1365	4.9679	13910.2
2900.	43.3429	4.9679	48.3109	4.9679	14407.0
3000.	43.5114	4.9679	48.4793	4.9679	14903.8
3100.	43.6743	4.9679	48.6422	4.9679	15400.6
3200.	43.8320	4.9679	48.7999	4.9679	15897.4
3300.	43.9849	4.9679	48.9528	4.9679	16394.2
3400.	44.1332	4.9679	49.1011	4.9679	16890.9
3500.	44.2772	4.9679	49.2451	4.9679	17387.7
3600.	44.4171	4.9679	49.3851	4.9679	17884.5
3700.	44.5532	4.9679	49.5212	4.9679	18381.3
3800.	44.6857	4.9679	49.6537	4.9679	18878.1
3900.	44.8148	4.9679	49.7827	4.9679	19374.9
4000.	44.9406	4.9679	49.9085	4.9679	19871.7
4100.	45.0632	4.9679	50.0311	4.9679	20368.5
4200.	45.1829	4.9679	50.1509	4.9679	20865.3
4300.	45.2998	4.9679	50.2678	4.9679	21362.1
4400.	45.4140	4.9679	50.3820	4.9679	21858.9
4500.	45.5257	4.9679	50.4936	4.9679	22355.7
4600.	45.6349	4.9679	50.6028	4.9679	22852.5
4700.	45.7417	4.9679	50.7096	4.9679	23349.2
4800.	45.8463	4.9679	50.8142	4.9679	23846.0
4900.	45.9487	4.9679	50.9167	4.9679	24342.8
5000.	46.0491	4.9679	51.0170	4.9679	24839.6
5100.	46.1475	4.9679	51.1154	4.9679	25336.4
5200.	46.2440	4.9679	51.2119	4.9679	25833.2
5300.	46.3386	4.9679	51.3065	4.9679	26330.0
5400.	46.4314	4.9679	51.3994	4.9679	26826.8
5500.	46.5226	4.9679	51.4905	4.9679	27323.6
5600.	46.6121	4.9679	51.5800	4.9679	27820.4
5700.	46.7000	4.9679	51.6680	4.9679	28317.2
5800.	46.7865	4.9679	51.7544	4.9679	28814.0
5900.	46.8714	4.9679	51.8393	4.9679	29310.8
6000.	46.9549	4.9679	51.9228	4.9679	29807.5

Talbe A-8-N Thermodynamic Functions for O^- - continued

T °K	$-\frac{(F^\circ-H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
6100.	47.0370	4.9679	52.0049	4.9679	30304.3
6200.	47.1178	4.9679	52.0857	4.9679	30801.1
6300.	47.1973	4.9679	52.1652	4.9679	31297.9
6400.	47.2755	4.9679	52.2434	4.9679	31794.7
6500.	47.3525	4.9679	52.3204	4.9679	32291.5
6600.	47.4284	4.9679	52.3963	4.9679	32788.3
6700.	47.5031	4.9679	52.4710	4.9679	33285.1
6800.	47.5767	4.9679	52.5446	4.9679	33781.9
6900.	47.6492	4.9679	52.6171	4.9679	34278.7
7000.	47.7207	4.9679	52.6886	4.9679	34775.5
7100.	47.7911	4.9679	52.7591	4.9679	35272.3
7200.	47.8606	4.9679	52.8286	4.9679	35769.1
7300.	47.9292	4.9679	52.8971	4.9679	36265.9
7400.	47.9967	4.9679	52.9647	4.9679	36762.6
7500.	48.0634	4.9679	53.0314	4.9679	37259.4
7600.	48.1292	4.9679	53.0972	4.9679	37756.2
7700.	48.1942	4.9679	53.1621	4.9679	38253.0
7800.	48.2583	4.9679	53.2262	4.9679	38749.8
7900.	48.3216	4.9679	53.2895	4.9679	39246.6
8000.	48.3841	4.9679	53.3520	4.9679	39743.4
8100.	48.4458	4.9679	53.4137	4.9679	40240.2
8200.	48.5067	4.9679	53.4746	4.9679	40737.0
8300.	48.5669	4.9679	53.5349	4.9679	41233.8
8400.	48.6264	4.9679	53.5944	4.9679	41730.6
8500.	48.6852	4.9679	53.6532	4.9679	42227.4
8600.	48.7433	4.9679	53.7113	4.9679	42724.2
8700.	48.8008	4.9679	53.7687	4.9679	43220.9
8800.	48.8575	4.9679	53.8255	4.9679	43717.7
8900.	48.9137	4.9679	53.8816	4.9679	44214.5
9000.	48.9692	4.9679	53.9371	4.9679	44711.3
9100.	49.0241	4.9679	53.9920	4.9679	45208.1
9200.	49.0784	4.9679	54.0463	4.9679	45704.9
9300.	49.1321	4.9679	54.1000	4.9679	46201.7
9400.	49.1852	4.9679	54.1531	4.9679	46698.5
9500.	49.2378	4.9679	54.2057	4.9679	47195.3
9600.	49.2898	4.9679	54.2577	4.9679	47692.1
9700.	49.3413	4.9679	54.3092	4.9679	48188.9
9800.	49.3922	4.9679	54.3602	4.9679	48685.7
9900.	49.4427	4.9679	54.4106	4.9679	49182.5
10000.	49.4926	4.9679	54.4605	4.9679	49679.2

Table A-9-N Thermodynamic Functions for F^-

T °K	$-\frac{(F^\circ - H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
273.15	29.3638	4.9679	34.3317	4.9679	1357.0
298.15	29.7989	4.9679	34.7668	4.9679	1481.2
1000.	35.8108	4.9679	40.7788	4.9679	4967.9
1100.	36.2843	4.9679	41.2522	4.9679	5464.7
1200.	36.7166	4.9679	41.6845	4.9679	5961.5
1300.	37.1142	4.9679	42.0822	4.9679	6458.3
1400.	37.4824	4.9679	42.4503	4.9679	6955.1
1500.	37.8252	4.9679	42.7931	4.9679	7451.9
1600.	38.1458	4.9679	43.1137	4.9679	7948.7
1700.	38.4470	4.9679	43.4149	4.9679	8445.5
1800.	38.7309	4.9679	43.6988	4.9679	8942.3
1900.	38.9995	4.9679	43.9674	4.9679	9439.1
2000.	39.2543	4.9679	44.2223	4.9679	9935.8
2100.	39.4967	4.9679	44.4646	4.9679	10432.6
2200.	39.7278	4.9679	44.6958	4.9679	10929.4
2300.	39.9487	4.9679	44.9166	4.9679	11426.2
2400.	40.1601	4.9679	45.1280	4.9679	11923.0
2500.	40.3629	4.9679	45.3308	4.9679	12419.8
2600.	40.5577	4.9679	45.5257	4.9679	12916.6
2700.	40.7452	4.9679	45.7132	4.9679	13413.4
2800.	40.9259	4.9679	45.8938	4.9679	13910.2
2900.	41.1002	4.9679	46.0682	4.9679	14407.0
3000.	41.2687	4.9679	46.2366	4.9679	14903.8
3100.	41.4316	4.9679	46.3995	4.9679	15400.6
3200.	41.5893	4.9679	46.5572	4.9679	15897.4
3300.	41.7421	4.9679	46.7101	4.9679	16394.2
3400.	41.8905	4.9679	46.8584	4.9679	16890.9
3500.	42.0345	4.9679	47.0024	4.9679	17387.7
3600.	42.1744	4.9679	47.1423	4.9679	17884.5
3700.	42.3105	4.9679	47.2785	4.9679	18381.3
3800.	42.4430	4.9679	47.4109	4.9679	18878.1
3900.	42.5721	4.9679	47.5400	4.9679	19374.9
4000.	42.6978	4.9679	47.6658	4.9679	19871.7
4100.	42.8205	4.9679	47.7884	4.9679	20368.5
4200.	42.9402	4.9679	47.9081	4.9679	20865.3
4300.	43.0571	4.9679	48.0250	4.9679	21362.1
4400.	43.1713	4.9679	48.1393	4.9679	21858.9
4500.	43.2830	4.9679	48.2509	4.9679	22355.7
4600.	43.3922	4.9679	48.3601	4.9679	22852.5
4700.	43.4990	4.9679	48.4669	4.9679	23349.2
4800.	43.6036	4.9679	48.5715	4.9679	23846.0
4900.	43.7060	4.9679	48.6740	4.9679	24342.8
5000.	43.8064	4.9679	48.7743	4.9679	24839.6
5100.	43.9048	4.9679	48.8727	4.9679	25336.4
5200.	44.0012	4.9679	48.9692	4.9679	25833.2
5300.	44.0959	4.9679	49.0638	4.9679	26330.0
5400.	44.1887	4.9679	49.1567	4.9679	26826.8
5500.	44.2799	4.9679	49.2478	4.9679	27323.6
5600.	44.3694	4.9679	49.3373	4.9679	27820.4
5700.	44.4573	4.9679	49.4253	4.9679	28317.2
5800.	44.5437	4.9679	49.5117	4.9679	28814.0
5900.	44.6287	4.9679	49.5966	4.9679	29310.8
6000.	44.7122	4.9679	49.6801	4.9679	29807.5

Table A-9-N Thermodynamic Functions for F^- - continued

T °K	$\frac{-(F^\circ - H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
6100.	44.7943	4.9679	49.7622	4.9679	30304.3
6200.	44.8751	4.9679	49.8430	4.9679	30801.1
6300.	44.9545	4.9679	49.9225	4.9679	31297.9
6400.	45.0328	4.9679	50.0007	4.9679	31794.7
6500.	45.1098	4.9679	50.0777	4.9679	32291.5
6600.	45.1857	4.9679	50.1536	4.9679	32788.3
6700.	45.2604	4.9679	50.2283	4.9679	33285.1
6800.	45.3340	4.9679	50.3019	4.9679	33781.9
6900.	45.4065	4.9679	50.3744	4.9679	34278.7
7000.	45.4780	4.9679	50.4459	4.9679	34775.5
7100.	45.5484	4.9679	50.5164	4.9679	35272.3
7200.	45.6179	4.9679	50.5858	4.9679	35769.1
7300.	45.6864	4.9679	50.6544	4.9679	36265.9
7400.	45.7540	4.9679	50.7220	4.9679	36762.6
7500.	45.8207	4.9679	50.7886	4.9679	37259.4
7600.	45.8865	4.9679	50.8544	4.9679	37756.2
7700.	45.9515	4.9679	50.9194	4.9679	38253.0
7800.	46.0156	4.9679	50.9835	4.9679	38749.8
7900.	46.0788	4.9679	51.0468	4.9679	39246.6
8000.	46.1413	4.9679	51.1093	4.9679	39743.4
8100.	46.2031	4.9679	51.1710	4.9679	40240.2
8200.	46.2640	4.9679	51.2319	4.9679	40737.0
8300.	46.3242	4.9679	51.2922	4.9679	41233.8
8400.	46.3837	4.9679	51.3516	4.9679	41730.6
8500.	46.4425	4.9679	51.4104	4.9679	42227.4
8600.	46.5006	4.9679	51.4685	4.9679	42724.2
8700.	46.5581	4.9679	51.5260	4.9679	43220.9
8800.	46.6148	4.9679	51.5828	4.9679	43717.7
8900.	46.6710	4.9679	51.6389	4.9679	44214.5
9000.	46.7265	4.9679	51.6944	4.9679	44711.3
9100.	46.7814	4.9679	51.7493	4.9679	45208.1
9200.	46.8357	4.9679	51.8036	4.9679	45704.9
9300.	46.8894	4.9679	51.8573	4.9679	46201.7
9400.	46.9425	4.9679	51.9104	4.9679	46698.5
9500.	46.9951	4.9679	51.9630	4.9679	47195.3
9600.	47.0471	4.9679	52.0150	4.9679	47692.1
9700.	47.0986	4.9679	52.0665	4.9679	48188.9
9800.	47.1495	4.9679	52.1175	4.9679	48685.7
9900.	47.2000	4.9679	52.1679	4.9679	49182.5
10000.	47.2499	4.9679	52.2178	4.9679	49679.2

Table A-17-N Thermodynamic Functions for Cl^-

T °K	$\frac{-(F^o - H^o_0)}{T}$	$\frac{H^o - H^o_0}{T}$	S^o	C^o_p	$H^o - H^o_0$
273.15	31.2233	4.9679	36.1912	4.9679	1357.0
298.15	31.6584	4.9679	36.6263	4.9679	1481.2
1000.	37.6703	4.9679	42.6383	4.9679	4967.9
1100.	38.1438	4.9679	43.1118	4.9679	5464.7
1200.	38.5761	4.9679	43.5440	4.9679	5961.5
1300.	38.9737	4.9679	43.9417	4.9679	6458.3
1400.	39.3419	4.9679	44.3098	4.9679	6955.1
1500.	39.6847	4.9679	44.6526	4.9679	7451.9
1600.	40.0053	4.9679	44.9732	4.9679	7948.7
1700.	40.3065	4.9679	45.2744	4.9679	8445.5
1800.	40.5904	4.9679	45.5583	4.9679	8942.3
1900.	40.8590	4.9679	45.8270	4.9679	9439.1
2000.	41.1138	4.9679	46.0818	4.9679	9935.8
2100.	41.3562	4.9679	46.3242	4.9679	10432.6
2200.	41.5873	4.9679	46.5553	4.9679	10929.4
2300.	41.8082	4.9679	46.7761	4.9679	11426.2
2400.	42.0196	4.9679	46.9875	4.9679	11923.0
2500.	42.2224	4.9679	47.1903	4.9679	12419.8
2600.	42.4173	4.9679	47.3852	4.9679	12916.6
2700.	42.6047	4.9679	47.5727	4.9679	13413.4
2800.	42.7854	4.9679	47.7533	4.9679	13910.2
2900.	42.9597	4.9679	47.9277	4.9679	14407.0
3000.	43.1282	4.9679	48.0961	4.9679	14903.8
3100.	43.2911	4.9679	48.2590	4.9679	15400.6
3200.	43.4488	4.9679	48.4167	4.9679	15897.4
3300.	43.6017	4.9679	48.5696	4.9679	16394.2
3400.	43.7500	4.9679	48.7179	4.9679	16890.9
3500.	43.8940	4.9679	48.8619	4.9679	17387.7
3600.	44.0339	4.9679	49.0019	4.9679	17884.5
3700.	44.1700	4.9679	49.1380	4.9679	18381.3
3800.	44.3025	4.9679	49.2705	4.9679	18878.1
3900.	44.4316	4.9679	49.3995	4.9679	19374.9
4000.	44.5574	4.9679	49.5253	4.9679	19871.7
4100.	44.6800	4.9679	49.6479	4.9679	20368.5
4200.	44.7997	4.9679	49.7677	4.9679	20865.3
4300.	44.9166	4.9679	49.8846	4.9679	21362.1
4400.	45.0308	4.9679	49.9988	4.9679	21858.9
4500.	45.1425	4.9679	50.1104	4.9679	22355.7
4600.	45.2517	4.9679	50.2196	4.9679	22852.5
4700.	45.3585	4.9679	50.3264	4.9679	23349.2
4800.	45.4631	4.9679	50.4310	4.9679	23846.0
4900.	45.5655	4.9679	50.5335	4.9679	24342.8
5000.	45.6659	4.9679	50.6338	4.9679	24839.6
5100.	45.7643	4.9679	50.7322	4.9679	25336.4
5200.	45.8608	4.9679	50.8287	4.9679	25833.2
5300.	45.9554	4.9679	50.9233	4.9679	26330.0
5400.	46.0482	4.9679	51.0162	4.9679	26826.8
5500.	46.1394	4.9679	51.1073	4.9679	27323.6
5600.	46.2289	4.9679	51.1968	4.9679	27820.4
5700.	46.3168	4.9679	51.2848	4.9679	28317.2
5800.	46.4032	4.9679	51.3712	4.9679	28814.0
5900.	46.4882	4.9679	51.4561	4.9679	29310.8
6000.	46.5717	4.9679	51.5396	4.9679	29807.5

Table A-17-N Thermodynamic Functions for Cl^- - continued

T °K	$\frac{-(F^\circ-H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
6100.	46.6538	4.9679	51.6217	4.9679	30304.3
6200.	46.7346	4.9679	51.7025	4.9679	30801.1
6300.	46.8141	4.9679	51.7820	4.9679	31297.9
6400.	46.8923	4.9679	51.8602	4.9679	31794.7
6500.	46.9693	4.9679	51.9372	4.9679	32291.5
6600.	47.0452	4.9679	52.0131	4.9679	32788.3
6700.	47.1199	4.9679	52.0878	4.9679	33285.1
6800.	47.1935	4.9679	52.1614	4.9679	33781.9
6900.	47.2660	4.9679	52.2339	4.9679	34278.7
7000.	47.3375	4.9679	52.3054	4.9679	34775.5
7100.	47.4079	4.9679	52.3759	4.9679	35272.3
7200.	47.4774	4.9679	52.4454	4.9679	35769.1
7300.	47.5460	4.9679	52.5139	4.9679	36265.9
7400.	47.6135	4.9679	52.5815	4.9679	36762.6
7500.	47.6802	4.9679	52.6482	4.9679	37259.4
7600.	47.7460	4.9679	52.7140	4.9679	37756.2
7700.	47.8110	4.9679	52.7789	4.9679	38253.0
7800.	47.8751	4.9679	52.8430	4.9679	38749.8
7900.	47.9384	4.9679	52.9063	4.9679	39246.6
8000.	48.0009	4.9679	52.9688	4.9679	39743.4
8100.	48.0626	4.9679	53.0305	4.9679	40240.2
8200.	48.1235	4.9679	53.0914	4.9679	40737.0
8300.	48.1837	4.9679	53.1517	4.9679	41233.8
8400.	48.2432	4.9679	53.2112	4.9679	41730.6
8500.	48.3020	4.9679	53.2700	4.9679	42227.4
8600.	48.3601	4.9679	53.3281	4.9679	42724.2
8700.	48.4176	4.9679	53.3855	4.9679	43220.9
8800.	48.4743	4.9679	53.4423	4.9679	43717.7
8900.	48.5305	4.9679	53.4984	4.9679	44214.5
9000.	48.5860	4.9679	53.5539	4.9679	44711.3
9100.	48.6409	4.9679	53.6088	4.9679	45208.1
9200.	48.6952	4.9679	53.6631	4.9679	45704.9
9300.	48.7489	4.9679	53.7168	4.9679	46201.7
9400.	48.8020	4.9679	53.7699	4.9679	46698.5
9500.	48.8546	4.9679	53.8225	4.9679	47195.3
9600.	48.9066	4.9679	53.8745	4.9679	47692.1
9700.	48.9581	4.9679	53.9260	4.9679	48188.9
9800.	49.0090	4.9679	53.9770	4.9679	48685.7
9900.	49.0595	4.9679	54.0274	4.9679	49182.5
10000.	49.1094	4.9679	54.0773	4.9679	49679.2

Table A-48-1 Thermodynamic Functions for N_2^+

T °K	$\frac{-(F^\circ - H_0^\circ)}{T}$	$\frac{H^\circ - H_0^\circ}{T}$	S°	C_p°	$H^\circ - H_0^\circ$
1000.	48.7433	7.2609	56.0044	7.9312	7260.9
1100.	49.4368	7.3281	56.7655	8.0623	8060.9
1200.	50.0787	7.3943	57.4729	8.1802	8873.1
1300.	50.6728	7.4588	58.1307	8.2883	9696.5
1400.	51.2273	7.5218	58.7487	8.3900	10530.6
1500.	51.7479	7.5828	59.3309	8.4886	11374.3
1600.	52.2407	7.6427	59.8834	8.5866	12228.2
1700.	52.7057	7.7011	60.4060	8.6857	13091.8
1800.	53.1469	7.7585	60.9048	8.7877	13965.3
1900.	53.5681	7.8155	61.3837	8.8926	14849.5
2000.	53.9695	7.8720	61.8427	9.0007	15744.0
2100.	54.3551	7.9284	62.2839	9.1120	16649.7
2200.	54.7267	7.9848	62.7111	9.2254	17566.7
2300.	55.0824	8.0413	63.1225	9.3405	18494.9
2400.	55.4261	8.0977	63.5239	9.4561	19434.5
2500.	55.7580	8.1544	63.9114	9.5714	20385.9
2600.	56.0779	8.2112	64.2889	9.6855	21349.1
2700.	56.3899	8.2678	64.6565	9.7971	22323.1
2800.	56.6900	8.3243	65.0142	9.9058	23307.9
2900.	56.9841	8.3807	65.3640	10.0106	24304.0
3000.	57.2683	8.4367	65.7058	10.1109	25310.2
3100.	57.5465	8.4922	66.0396	10.2061	26325.7
3200.	57.8167	8.5472	66.3635	10.2961	27351.1
3300.	58.0810	8.6015	66.6815	10.3804	28384.8
3400.	58.3373	8.6549	66.9935	10.4587	29426.7
3500.	58.5897	8.7076	67.2975	10.5310	30476.5
3600.	58.8361	8.7592	67.5956	10.5974	31533.3
3700.	59.0766	8.8097	67.8857	10.6580	32596.0
3800.	59.3130	8.8590	68.1719	10.7126	33664.2
3900.	59.5436	8.9073	68.4501	10.7619	34738.4
4000.	59.7701	8.9542	68.7223	10.8056	35816.8
4100.	59.9907	8.9999	68.9906	10.8442	36899.6
4200.	60.2073	9.0442	69.2529	10.8780	37985.7
4300.	60.4219	9.0871	69.5092	10.9074	39074.7
4400.	60.6305	9.1289	69.7596	10.9322	40167.0
4500.	60.8372	9.1692	70.0060	10.9533	41261.4
4600.	61.0379	9.2081	70.2465	10.9706	42357.5
4700.	61.2366	9.2457	70.4829	10.9845	43454.8
4800.	61.4314	9.2821	70.7134	10.9954	44553.9
4900.	61.6241	9.3170	70.9400	11.0036	45653.5
5000.	61.8129	9.3508	71.1625	11.0091	46754.1
5100.	61.9977	9.3834	71.3811	11.0123	47855.4
5200.	62.1805	9.4148	71.5957	11.0135	48957.0
5300.	62.3594	9.4450	71.8044	11.0129	50058.6

Table A-48-1 Thermodynamic Functions for N_2^+ - continued

T °K	$\frac{-(F^\circ - H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
5400.	62.5362	9.4740	72.0111	11.0107	51159.8
5500.	62.7111	9.5019	72.2118	11.0071	52260.2
5600.	62.8820	9.5287	72.4105	11.0024	53360.6
5700.	63.0509	9.5545	72.6052	10.9966	54460.7
5800.	63.2178	9.5794	72.7960	10.9898	55560.2
5900.	63.3808	9.6032	72.9848	10.9825	56658.9
6000.	63.5437	9.6261	73.1696	10.9743	57756.3
6100.	63.7027	9.6481	73.3504	10.9658	58853.5
6200.	63.8597	9.6694	73.5293	10.9569	59950.1
6300.	64.0147	9.6896	73.7041	10.9475	61044.7
6400.	64.1677	9.7093	73.8770	10.9382	62139.6
6500.	64.3167	9.7282	74.0459	10.9286	63233.2
6600.	64.4658	9.7463	74.2128	10.9191	64325.4
6700.	64.6128	9.7636	74.3758	10.9096	65415.9
6800.	64.7579	9.7805	74.5387	10.9002	66507.1
6900.	64.9010	9.7965	74.6977	10.8909	67596.2
7000.	65.0421	9.8122	74.8547	10.8819	68685.7
7100.	65.1812	9.8272	75.0077	10.8730	69772.8
7200.	65.3183	9.8417	75.1607	10.8645	70859.9
7300.	65.4554	9.8556	75.3098	10.8561	71945.6
7400.	65.5885	9.8691	75.4568	10.8482	73031.2
7500.	65.7217	9.8820	75.6039	10.8404	74115.0
7600.	65.8528	9.8947	75.7469	10.8333	75199.8
7700.	65.9820	9.9068	75.8880	10.8263	76282.6
7800.	66.1092	9.9186	76.0271	10.8197	77364.8
7900.	66.2363	9.9299	76.1662	10.8136	78446.1
8000.	66.3615	9.9408	76.3014	10.8078	79526.5
8100.	66.4847	9.9515	76.4365	10.8025	80607.5
8200.	66.6060	9.9619	76.5676	10.7977	81687.4
8300.	66.7272	9.9720	76.6988	10.7931	82767.7
8400.	66.8464	9.9818	76.8280	10.7889	83846.7
8500.	66.9656	9.9911	76.9571	10.7852	84924.3
8600.	67.0829	10.0004	77.0823	10.7816	86003.7
8700.	67.1981	10.0094	77.2075	10.7786	87081.6
8800.	67.3114	10.0181	77.3307	10.7758	88159.4
8900.	67.4247	10.0267	77.4519	10.7736	89237.3
9000.	67.5379	10.0348	77.5732	10.7715	90313.3
9100.	67.6492	10.0430	77.6924	10.7699	91390.9
9200.	67.7585	10.0509	77.8096	10.7683	92468.3
9300.	67.8678	10.0585	77.9249	10.7673	93543.7
9400.	67.9751	10.0660	78.0401	10.7663	94620.5
9500.	68.0804	10.0734	78.1554	10.7657	95696.9
9600.	68.1858	10.0807	78.2667	10.7653	96774.9
9700.	68.2911	10.0877	78.3780	10.7651	97850.4
9800.	68.3944	10.0946	78.4892	10.7651	98927.3
9900.	68.4977	10.1014	78.5985	10.7653	100003.7
10000.	68.5991	10.1081	78.7058	10.7657	101081.4

Table A-83-1 Thermodynamic Functions for O_2^+

T °K	$\frac{-(F^\circ - H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
1000.	50.8636	7.3827	58.2459	8.1524	7382.7
1100.	51.5710	7.4580	59.0289	8.2686	8203.9
1200.	52.2228	7.5298	59.7522	8.3672	9035.7
1300.	52.8289	7.5975	60.4259	8.4508	9876.8
1400.	53.3933	7.6611	61.0558	8.5224	10725.6
1500.	53.9238	7.7206	61.6460	8.5840	11580.8
1600.	54.4246	7.7764	62.2004	8.6376	12442.2
1700.	54.8976	7.8285	62.7270	8.6843	13308.4
1800.	55.3467	7.8771	63.2238	8.7257	14178.9
1900.	55.7739	7.9228	63.6967	8.7626	15053.4
2000.	56.1813	7.9656	64.1458	8.7956	15931.1
2100.	56.5708	8.0059	64.5771	8.8254	16812.4
2200.	56.9443	8.0437	64.9884	8.8524	17696.1
2300.	57.3020	8.0794	65.3819	8.8775	18582.7
2400.	57.6478	8.1132	65.7594	8.9005	19471.7
2500.	57.9797	8.1450	66.1231	8.9220	20362.5
2600.	58.2996	8.1754	66.4748	8.9421	21256.1
2700.	58.6076	8.2040	66.8126	8.9609	22150.9
2800.	58.9077	8.2315	67.1385	8.9790	23048.1
2900.	59.1958	8.2575	67.4545	8.9961	23946.7
3000.	59.4760	8.2825	67.7585	9.0128	24847.6
3100.	59.7482	8.3062	68.0546	9.0287	25749.1
3200.	60.0125	8.3290	68.3408	9.0444	26652.9
3300.	60.2689	8.3511	68.6210	9.0599	27558.6
3400.	60.5193	8.3721	68.8912	9.0752	28465.3
3500.	60.7617	8.3924	69.1535	9.0905	29373.5
3600.	60.9982	8.4119	69.4099	9.1060	30282.8
3700.	61.2287	8.4310	69.6602	9.1215	31194.6
3800.	61.4552	8.4492	69.9027	9.1376	32107.1
3900.	61.6738	8.4671	70.1411	9.1541	33021.8
4000.	61.8884	8.4846	70.3736	9.1714	33938.5
4100.	62.0991	8.5015	70.6002	9.1893	34856.2
4200.	62.3037	8.5182	70.8208	9.2081	35776.5
4300.	62.5044	8.5345	71.0393	9.2278	36698.3
4400.	62.7012	8.5504	71.2500	9.2489	37621.7
4500.	62.8919	8.5661	71.4586	9.2711	38547.4
4600.	63.0807	8.5818	71.6633	9.2946	39476.2
4700.	63.2655	8.5971	71.8640	9.3198	40406.3
4800.	63.4464	8.6126	72.0588	9.3467	41340.4
4900.	63.6252	8.6277	72.2535	9.3751	42275.7
5000.	63.8001	8.6430	72.4423	9.4055	43215.0
5100.	63.9710	8.6583	72.6291	9.4377	44157.3
5200.	64.1379	8.6736	72.8119	9.4718	45102.7
5300.	64.3048	8.6891	72.9927	9.5082	46052.2

Table A-83-1 Thermodynamic Functions for O_2^+ - continued

T °K	$\frac{-(F^\circ-H_0^\circ)}{T}$	$\frac{H^\circ - H_0^\circ}{T}$	S°	C_p°	$H^\circ - H_0^\circ$
5400.	64.4658	8.7046	73.1716	9.5468	47004.8
5500.	64.6267	8.7203	73.3464	9.5875	47961.6
5600.	64.7837	8.7360	73.5193	9.6306	48921.6
5700.	64.9387	8.7521	73.6902	9.6759	49886.9
5800.	65.0917	8.7686	73.8591	9.7234	50857.8
5900.	65.2408	8.7851	74.0261	9.7733	51832.0
6000.	65.3898	8.8020	74.1910	9.8256	52811.8
6100.	65.5349	8.8193	74.3539	9.8802	53797.5
6200.	65.6780	8.8367	74.5149	9.9372	54787.8
6300.	65.8190	8.8548	74.6739	9.9963	55785.4
6400.	65.9601	8.8731	74.8328	10.0577	56787.9
6500.	66.0972	8.8918	74.9878	10.1215	57796.6
6600.	66.2324	8.9109	75.1428	10.1870	58811.7
6700.	66.3675	8.9305	75.2978	10.2548	59834.6
6800.	66.4987	8.9504	75.4489	10.3245	60862.8
6900.	66.6298	8.9709	75.6019	10.3963	61899.1
7000.	66.7590	8.9917	75.7509	10.4696	62942.2
7100.	66.8862	9.0130	75.9000	10.5447	63992.4
7200.	67.0133	9.0349	76.0490	10.6214	65051.0
7300.	67.1385	9.0571	76.1960	10.6997	66117.0
7400.	67.2617	9.0800	76.3411	10.7792	67191.8
7500.	67.3829	9.1030	76.4862	10.8599	68272.7
7600.	67.5042	9.1267	76.6312	10.9418	69362.7
7700.	67.6234	9.1509	76.7743	11.0244	70462.1
7800.	67.7426	9.1754	76.9174	11.1081	71567.8
7900.	67.8599	9.2004	77.0585	11.1923	72683.1
8000.	67.9751	9.2258	77.2016	11.2772	73806.7
8100.	68.0904	9.2517	77.3407	11.3624	74938.5
8200.	68.2036	9.2779	77.4817	11.4481	76078.8
8300.	68.3169	9.3045	77.6208	11.5337	77227.6
8400.	68.4282	9.3318	77.7599	11.6194	78386.7
8500.	68.5375	9.3590	77.8971	11.7048	79551.3
8600.	68.6468	9.3868	78.0342	11.7901	80726.4
8700.	68.7561	9.4150	78.1713	11.8747	81910.6
8800.	68.8634	9.4434	78.3084	11.9590	83102.2
8900.	68.9707	9.4720	78.4435	12.0424	84301.2
9000.	69.0780	9.5011	78.5787	12.1251	85509.5
9100.	69.1813	9.5305	78.7118	12.2070	86727.2
9200.	69.2867	9.5599	78.8469	12.2877	87950.9
9300.	69.3900	9.5897	78.9801	12.3672	89184.1
9400.	69.4933	9.6197	79.1132	12.4454	90425.1
9500.	69.5947	9.6499	79.2444	12.5222	91674.0
9600.	69.6960	9.6801	79.3755	12.5975	92929.0
9700.	69.7974	9.7105	79.5067	12.6712	94191.9
9800.	69.8967	9.7411	79.6378	12.7433	95462.8
9900.	69.9961	9.7719	79.7670	12.8135	96741.9
10000.	70.0934	9.8027	79.8962	12.8818	98027.1

Table A-89-1 Thermodynamic Functions for NO+

T °K	$\frac{-(F^\circ-H^\circ_0)}{T}$	$\frac{H^\circ - H^\circ_0}{T}$	S°	C°_p	$H^\circ - H^\circ_0$
1000.	48.9519	7.2114	56.1634	7.8239	7211.4
1100.	49.6415	7.2732	56.9165	7.9540	8000.6
1200.	50.2774	7.3348	57.6120	8.0691	8801.8
1300.	50.8676	7.3953	58.2618	8.1701	9613.8
1400.	51.4180	7.4539	58.8719	8.2587	10435.4
1500.	51.9347	7.5101	59.4442	8.3360	11265.2
1600.	52.4196	7.5640	59.9847	8.4039	12102.3
1700.	52.8806	7.6152	60.4954	8.4638	12945.9
1800.	53.3178	7.6637	60.9803	8.5166	13794.7
1900.	53.7331	7.7100	61.4433	8.5635	14649.0
2000.	54.1285	7.7537	61.8825	8.6052	15507.5
2100.	54.5081	7.7951	62.3037	8.6428	16369.7
2200.	54.8717	7.8344	62.7071	8.6764	17235.7
2300.	55.2215	7.8718	63.0926	8.7070	18105.1
2400.	55.5573	7.9071	63.4642	8.7346	18977.2
2500.	55.8812	7.9407	63.8219	8.7598	19851.8
2600.	56.1932	7.9727	64.1657	8.7829	20729.1
2700.	56.4933	8.0031	64.4976	8.8044	21608.4
2800.	56.7854	8.0321	64.8175	8.8240	22490.0
2900.	57.0675	8.0598	65.1275	8.8423	23373.3
3000.	57.3418	8.0860	65.4276	8.8594	24258.0
3100.	57.6081	8.1112	65.7177	8.8753	25144.8
3200.	57.8644	8.1355	65.9999	8.8904	26033.5
3300.	58.1148	8.1585	66.2741	8.9045	26923.1
3400.	58.3592	8.1806	66.5404	8.9178	27814.0
3500.	58.5977	8.2018	66.7987	8.9305	28706.5
3600.	58.8282	8.2223	67.0511	8.9427	29600.3
3700.	59.0547	8.2420	67.2955	8.9542	30495.3
3800.	59.2733	8.2609	67.5340	8.9653	31391.3
3900.	59.4879	8.2789	67.7685	8.9760	32287.9
4000.	59.6986	8.2966	67.9950	8.9862	33186.5
4100.	59.9032	8.3135	68.2176	8.9961	34085.4
4200.	60.1039	8.3298	68.4342	9.0059	34985.2
4300.	60.3007	8.3457	68.6468	9.0152	35886.6
4400.	60.4934	8.3610	68.8535	9.0241	36788.5
4500.	60.6802	8.3759	69.0561	9.0331	37691.6
4600.	60.8650	8.3902	69.2549	9.0416	38595.1
4700.	61.0459	8.4041	69.4496	9.0502	39499.5
4800.	61.2227	8.4177	69.6404	9.0585	40404.7
4900.	61.3956	8.4310	69.8272	9.0667	41311.7
5000.	61.5665	8.4437	70.0100	9.0746	42218.4
5100.	61.7334	8.4562	70.1908	9.0826	43126.6
5200.	61.8984	8.4683	70.3657	9.0903	44035.3
5300.	62.0593	8.4800	70.5406	9.0981	44944.3

Table A-89-1 Thermodynamic Functions for NO+ - continued

T °K	$-(F^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C°_p	$H^\circ - H^\circ_0$
5400.	62.2183	8.4916	70.7095	9.1058	45854.5
5500.	62.3733	8.5029	70.8764	9.1134	46766.0
5600.	62.5283	8.5138	71.0413	9.1209	47677.5
5700.	62.6773	8.5246	71.2023	9.1283	48590.0
5800.	62.8264	8.5349	71.3613	9.1358	49502.4
5900.	62.9734	8.5452	71.5182	9.1432	50416.8
6000.	63.1165	8.5552	71.6713	9.1507	51331.0
6100.	63.2576	8.5651	71.8223	9.1581	52247.1
6200.	63.3967	8.5746	71.9713	9.1654	53162.8
6300.	63.5338	8.5842	72.1184	9.1730	54080.3
6400.	63.6689	8.5933	72.2634	9.1803	54997.2
6500.	63.8021	8.6025	72.4045	9.1877	55916.0
6600.	63.9352	8.6114	72.5456	9.1952	56835.2
6700.	64.0644	8.6201	72.6847	9.2028	57755.0
6800.	64.1916	8.6289	72.8198	9.2103	58676.4
6900.	64.3187	8.6372	72.9550	9.2179	59596.9
7000.	64.4419	8.6456	73.0881	9.2256	60519.1
7100.	64.5651	8.6539	73.2193	9.2334	61442.9
7200.	64.6864	8.6619	73.3484	9.2411	62365.5
7300.	64.8056	8.6700	73.4756	9.2491	63291.2
7400.	64.9228	8.6778	73.6008	9.2570	64215.5
7500.	65.0401	8.6855	73.7260	9.2650	65141.4
7600.	65.1553	8.6933	73.8492	9.2731	66068.9
7700.	65.2686	8.7008	73.9704	9.2815	66996.3
7800.	65.3819	8.7084	74.0896	9.2898	67925.3
7900.	65.4912	8.7157	74.2069	9.2982	68854.2
8000.	65.6024	8.7231	74.3241	9.3067	69784.6
8100.	65.7097	8.7304	74.4414	9.3155	70716.5
8200.	65.8171	8.7376	74.5546	9.3244	71648.2
8300.	65.9224	8.7447	74.6679	9.3333	72581.3
8400.	66.0277	8.7517	74.7792	9.3425	73514.2
8500.	66.1310	8.7587	74.8905	9.3516	74448.5
8600.	66.2344	8.7656	74.9998	9.3612	75384.2
8700.	66.3357	8.7726	75.1091	9.3707	76321.3
8800.	66.4351	8.7795	75.2144	9.3804	77259.7
8900.	66.5344	8.7863	75.3217	9.3904	78197.8
9000.	66.6338	8.7930	75.4270	9.4003	79137.3
9100.	66.7312	8.7998	75.5303	9.4106	80078.0
9200.	66.8265	8.8063	75.6337	9.4210	81018.4
9300.	66.9219	8.8131	75.7350	9.4315	81961.8
9400.	67.0153	8.8197	75.8364	9.4422	82904.8
9500.	67.1087	8.8264	75.9357	9.4534	83850.9
9600.	67.2021	8.8330	76.0351	9.4645	84796.5
9700.	67.2935	8.8395	76.1325	9.4758	85743.4
9800.	67.3849	8.8461	76.2298	9.4871	86691.6
9900.	67.4744	8.8526	76.3272	9.4989	87641.2
10000.	67.5638	8.8592	76.4226	9.5108	88592.0

Table A-51 REVISED. Thermodynamic Functions for BeF_2(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	44.745	8.637	53.382	10.769	2359.3	54.379
298.15	45.509	8.827	54.336	11.028	2631.8	54.336
50.00	32.085	6.954	39.039	6.989	347.7	84.721
75.00	34.912	7.005	41.917	7.280	525.4	70.002
100.00	36.943	7.138	44.082	7.820	713.8	63.261
125.00	38.556	7.334	45.890	8.408	916.7	59.611
150.00	39.913	7.558	47.472	8.945	1133.8	57.458
175.00	41.096	7.791	48.887	9.416	1363.4	56.134
200.00	42.151	8.020	50.171	9.826	1604.1	55.310
225.00	43.109	8.241	51.350	10.185	1854.3	54.805
250.00	43.988	8.452	52.440	10.504	2113.0	54.515
275.00	44.803	8.652	53.455	10.789	2379.2	54.373
300.00	45.564	8.841	54.405	11.047	2652.2	54.336
325.00	46.279	9.020	55.298	11.282	2931.4	54.376
350.00	46.953	9.189	56.142	11.498	3216.1	54.473
375.00	47.593	9.350	56.942	11.697	3506.1	54.611
400.00	48.201	9.502	57.703	11.882	3800.9	54.781
425.00	48.782	9.647	58.429	12.055	4100.1	54.974
450.00	49.337	9.786	59.123	12.216	4403.5	55.185
475.00	49.870	9.918	59.787	12.366	4710.8	55.410
500.00	50.381	10.043	60.425	12.507	5021.7	55.645
550.00	51.350	10.279	61.629	12.760	5653.6	56.135
600.00	52.254	10.495	62.749	12.982	6297.3	56.640
650.00	53.102	10.694	63.796	13.176	6951.3	57.151
700.00	53.901	10.878	64.779	13.346	7614.5	57.661
750.00	54.658	11.047	65.705	13.494	8285.5	58.167
800.00	55.376	11.204	66.580	13.625	8963.6	58.665
850.00	56.059	11.350	67.410	13.739	9647.7	59.155
900.00	56.712	11.486	68.198	13.840	10337.3	59.636
950.00	57.336	11.612	68.949	13.930	11031.6	60.107
1000.00	57.935	11.730	69.665	14.009	11730.1	60.567
1050.00	58.510	11.840	70.350	14.079	12432.3	61.016
1100.00	59.063	11.944	71.007	14.142	13137.9	61.456
1150.00	59.596	12.040	71.637	14.199	13846.4	61.885
1200.00	60.111	12.131	72.242	14.249	14557.7	62.304
1250.00	60.608	12.217	72.825	14.295	15271.3	62.713
1300.00	61.088	12.298	73.386	14.336	15987.1	63.113
1350.00	61.554	12.374	73.928	14.373	16704.8	63.503
1400.00	62.005	12.446	74.451	14.407	17424.4	63.885
1450.00	62.443	12.514	74.957	14.438	18145.5	64.258
1500.00	62.869	12.579	75.447	14.466	18868.1	64.623
1550.00	63.282	12.640	75.922	14.492	19592.1	64.980
1600.00	63.684	12.698	76.383	14.515	20317.2	65.329
1650.00	64.076	12.754	76.830	14.537	21043.6	65.671
1700.00	64.457	12.806	77.264	14.557	21770.9	66.006
1750.00	64.829	12.857	77.686	14.575	22499.2	66.333
1800.00	65.192	12.905	78.097	14.592	23228.4	66.654
1850.00	65.546	12.950	78.497	14.608	23958.4	66.969
1900.00	65.892	12.994	78.887	14.622	24689.2	67.278
1950.00	66.230	13.036	79.267	14.636	25420.6	67.580
2000.00	66.561	13.076	79.637	14.649	26152.7	67.877
2050.00	66.884	13.115	79.999	14.660	26885.5	68.168

Table A-51 REVISED. Thermodynamic Functions for BeF_2(gas)-Continued

2100.00	67.201	13.152	80.353	14.671	27618.8	68.454
2150.00	67.511	13.187	80.698	14.682	28352.6	68.735
2200.00	67.814	13.221	81.036	14.691	29086.9	69.011
2250.00	68.112	13.254	81.366	14.700	29821.7	69.281
2300.00	68.403	13.286	81.689	14.709	30556.9	69.548
2350.00	68.690	13.316	82.005	14.717	31292.5	69.809
2400.00	68.970	13.345	82.315	14.724	32028.5	70.067
2450.00	69.246	13.373	82.619	14.731	32764.9	70.320
2500.00	69.516	13.401	82.917	14.738	33501.6	70.569
2600.00	70.043	13.452	83.495	14.750	34976.0	71.055
2700.00	70.551	13.501	84.052	14.761	36451.6	71.526
2800.00	71.043	13.546	84.589	14.771	37928.1	71.983
2900.00	71.519	13.588	85.107	14.779	39405.6	72.427
3000.00	71.981	13.628	85.609	14.787	40884.0	72.858
3100.00	72.428	13.666	86.094	14.795	42363.1	73.277
3200.00	72.862	13.701	86.563	14.801	43842.9	73.685
3300.00	73.285	13.734	87.019	14.807	45323.3	74.082
3400.00	73.695	13.766	87.461	14.813	46804.3	74.469
3500.00	74.095	13.796	87.890	14.818	48285.8	74.846
3600.00	74.484	13.824	88.308	14.822	49767.8	75.215
3700.00	74.863	13.851	88.714	14.827	51250.3	75.574
3800.00	75.232	13.877	89.110	14.831	52733.1	75.925
3900.00	75.593	13.902	89.495	14.834	54216.4	76.268
4000.00	75.945	13.925	89.870	14.838	55700.0	76.603
4100.00	76.290	13.947	90.237	14.841	57183.9	76.932
4200.00	76.626	13.969	90.595	14.844	58668.1	77.253
4300.00	76.955	13.989	90.944	14.846	60152.6	77.567
4400.00	77.277	14.009	91.285	14.849	61637.4	77.875
4500.00	77.592	14.027	91.619	14.851	63122.4	78.177
4600.00	77.900	14.045	91.945	14.854	64607.7	78.472
4700.00	78.202	14.062	92.265	14.856	66093.2	78.762
4800.00	78.499	14.079	92.578	14.858	67578.8	79.047
4900.00	78.789	14.095	92.884	14.860	69064.7	79.326
5000.00	79.074	14.110	93.184	14.861	70550.7	79.600
5100.00	79.354	14.125	93.479	14.863	72037.0	79.870
5200.00	79.628	14.139	93.767	14.864	73523.3	80.134
5300.00	79.898	14.153	94.050	14.866	75009.8	80.394
5400.00	80.162	14.166	94.328	14.867	76496.5	80.650
5500.00	80.422	14.179	94.601	14.869	77983.3	80.901
5600.00	80.678	14.191	94.869	14.870	79470.2	81.148
5700.00	80.929	14.203	95.132	14.871	80957.3	81.391
5800.00	81.176	14.215	95.391	14.872	82444.4	81.630
5900.00	81.419	14.226	95.645	14.873	83931.7	81.865
6000.00	81.659	14.237	95.895	14.874	85419.1	82.097

This table was computed for the ground electronic state (assumed to be $^1\Sigma$) in the harmonic oscillator-rigid rotator approximation using a molecular weight of 47.0090 and the following molecular constants: moment of inertia, 68.227 (in atomic-weight units and Å); symmetry number, 2; frequencies (in cm^{-1}) and degeneracies, 750(1), 320(2), 1535(1). (See p. 123 and Chapter B-7, p. 85.)

Table A-90. Thermodynamic Functions for BeOAℓ(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	51.359	8.892	60.251	9.955	2428.8	61.169
298.15	52.142	8.988	61.130	10.120	2679.7	61.130
50.00	37.324	7.950	45.273	7.994	397.5	90.918
75.00	40.554	7.999	48.554	8.234	600.0	76.284
100.00	42.868	8.100	50.968	8.567	810.0	69.666
125.00	44.689	8.224	52.913	8.867	1028.0	66.127
150.00	46.200	8.352	54.552	9.108	1252.8	64.065
175.00	47.497	8.475	55.971	9.306	1483.1	62.809
200.00	48.636	8.590	57.225	9.479	1717.9	62.034
225.00	49.654	8.698	58.351	9.643	1957.0	61.564
250.00	50.576	8.800	59.376	9.804	2200.1	61.294
275.00	51.419	8.899	60.318	9.967	2447.2	61.163
300.00	52.197	8.995	61.192	10.133	2698.4	61.130
325.00	52.921	9.089	62.010	10.299	2953.8	61.166
350.00	53.598	9.181	62.779	10.465	3213.4	61.254
375.00	54.235	9.272	63.507	10.630	3477.1	61.380
400.00	54.836	9.362	64.198	10.791	3744.9	61.535
425.00	55.406	9.451	64.857	10.948	4016.6	61.711
450.00	55.949	9.538	65.487	11.099	4292.2	61.904
475.00	56.467	9.624	66.091	11.244	4571.5	62.108
500.00	56.963	9.709	66.671	11.383	4854.4	62.322
550.00	57.896	9.873	67.768	11.639	5430.0	62.768
600.00	58.762	10.030	68.791	11.867	6017.8	63.228
650.00	59.570	10.179	69.749	12.069	6616.3	63.693
700.00	60.330	10.320	70.650	12.248	7224.3	64.158
750.00	61.046	10.454	71.501	12.405	7840.7	64.619
800.00	61.725	10.581	72.306	12.544	8464.5	65.075
850.00	62.370	10.700	73.070	12.666	9094.9	65.523
900.00	62.985	10.812	73.797	12.774	9730.9	65.963
950.00	63.573	10.918	74.491	12.869	10372.1	66.393
1000.00	64.135	11.018	75.153	12.954	11017.7	66.815
1050.00	64.675	11.112	75.787	13.030	11667.3	67.227
1100.00	65.194	11.200	76.394	13.097	12320.5	67.630
1150.00	65.694	11.284	76.978	13.157	12976.9	68.024
1200.00	66.176	11.363	77.539	13.211	13636.1	68.409
1250.00	66.641	11.438	78.079	13.260	14298.0	68.785
1300.00	67.091	11.509	78.600	13.304	14962.1	69.152
1350.00	67.527	11.577	79.103	13.344	15628.3	69.512
1400.00	67.949	11.640	79.589	13.380	16296.4	69.863
1450.00	68.358	11.701	80.059	13.413	16966.3	70.207
1500.00	68.756	11.758	80.515	13.443	17637.7	70.543
1550.00	69.143	11.813	80.956	13.471	18310.5	70.871
1600.00	69.518	11.865	81.384	13.496	18984.7	71.193
1650.00	69.884	11.915	81.800	13.519	19660.1	71.508
1700.00	70.241	11.963	82.203	13.540	20336.5	71.817
1750.00	70.588	12.008	82.596	13.560	21014.0	72.119
1800.00	70.927	12.051	82.978	13.578	21692.5	72.416
1850.00	71.258	12.093	83.351	13.595	22371.8	72.706
1900.00	71.581	12.133	83.713	13.610	23051.9	72.991
1950.00	71.896	12.171	84.067	13.625	23732.8	73.271
2000.00	72.205	12.207	84.412	13.638	24414.4	73.545
2050.00	72.507	12.242	84.749	13.651	25096.6	73.814

Table A-90. Thermodynamic Functions for BeOAl(gas)-Continued

2100.00	72.802	12.276	85.078	13.662	25779.4	74.078
2150.00	73.092	12.308	85.400	13.673	26462.8	74.338
2200.00	73.375	12.339	85.714	13.684	27146.7	74.593
2250.00	73.653	12.369	86.022	13.693	27831.1	74.844
2300.00	73.925	12.398	86.323	13.702	28516.0	75.090
2350.00	74.192	12.426	86.618	13.711	29201.4	75.332
2400.00	74.454	12.453	86.907	13.719	29887.1	75.570
2450.00	74.711	12.479	87.189	13.726	30573.2	75.804
2500.00	74.963	12.504	87.467	13.733	31259.7	76.035
2600.00	75.454	12.551	88.006	13.746	32633.7	76.485
2700.00	75.929	12.596	88.525	13.758	34008.9	76.921
2800.00	76.388	12.638	89.025	13.768	35385.2	77.345
2900.00	76.832	12.677	89.509	13.778	36762.5	77.756
3000.00	77.262	12.714	89.976	13.786	38140.7	78.155
3100.00	77.680	12.748	90.428	13.794	39519.7	78.544
3200.00	78.085	12.781	90.866	13.801	40899.4	78.922
3300.00	78.479	12.812	91.291	13.807	42279.8	79.291
3400.00	78.862	12.841	91.703	13.813	43660.9	79.650
3500.00	79.234	12.869	92.104	13.819	45042.4	80.000
3600.00	79.597	12.896	92.493	13.823	46424.5	80.342
3700.00	79.951	12.921	92.872	13.828	47807.1	80.675
3800.00	80.296	12.945	93.241	13.832	49190.1	81.001
3900.00	80.632	12.968	93.600	13.836	50573.6	81.319
4000.00	80.961	12.989	93.950	13.840	51957.4	81.631
4100.00	81.282	13.010	94.292	13.843	53341.5	81.936
4200.00	81.596	13.030	94.626	13.846	54726.0	82.234
4300.00	81.903	13.049	94.952	13.849	56110.8	82.526
4400.00	82.203	13.067	95.270	13.852	57495.8	82.812
4500.00	82.497	13.085	95.581	13.854	58881.1	83.092
4600.00	82.784	13.101	95.886	13.857	60266.7	83.367
4700.00	83.066	13.118	96.184	13.859	61652.5	83.636
4800.00	83.343	13.133	96.476	13.861	63038.5	83.901
4900.00	83.614	13.148	96.761	13.863	64424.7	84.160
5000.00	83.879	13.162	97.042	13.865	65811.1	84.415
5100.00	84.140	13.176	97.316	13.867	67197.7	84.666
5200.00	84.396	13.189	97.585	13.868	68584.4	84.911
5300.00	84.647	13.202	97.850	13.870	69971.3	85.153
5400.00	84.894	13.215	98.109	13.871	71358.4	85.391
5500.00	85.137	13.226	98.363	13.873	72745.6	85.624
5600.00	85.375	13.238	98.613	13.874	74132.9	85.854
5700.00	85.610	13.249	98.859	13.875	75520.4	86.080
5800.00	85.840	13.260	99.100	13.876	76908.0	86.302
5900.00	86.067	13.270	99.337	13.878	78295.7	86.521
6000.00	86.290	13.281	99.571	13.879	79683.5	86.737

This table was computed for the ground electronic state (assumed to be $^2\Sigma$) in the harmonic oscillator-rigid rotator approximation using a molecular weight of 51.9931 and the following molecular constants: moments of inertia (in atomic-weight units and Å), $I_A = 66.397$, $I_B = 67.834$, $I_C = 1.436$; symmetry number, 1; frequencies (in cm^{-1}) and degeneracies, 1500(1), 1000(1), 275(1). (See p. 123 and Chapter B-7, p. 85.)

Table A-91. Thermodynamic Functions for LiH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	33.236	6.929	40.165	7.014	1892.7	40.809
298.15	33.843	6.938	40.781	7.056	2068.6	40.781
50.00	21.550	6.810	28.361	6.952	340.5	62.922
75.00	24.322	6.857	31.179	6.949	514.3	51.903
100.00	26.298	6.880	33.178	6.947	688.0	46.984
125.00	27.835	6.893	34.728	6.945	861.6	44.383
150.00	29.092	6.902	35.994	6.944	1035.2	42.883
175.00	30.157	6.908	37.064	6.944	1208.8	41.977
200.00	31.079	6.912	37.992	6.950	1382.5	41.422
225.00	31.894	6.917	38.811	6.963	1556.4	41.087
250.00	32.623	6.923	39.546	6.985	1730.7	40.897
275.00	33.283	6.930	40.213	7.017	1905.7	40.805
300.00	33.886	6.939	40.825	7.059	2081.6	40.782
325.00	34.442	6.950	41.392	7.110	2258.7	40.807
350.00	34.958	6.963	41.921	7.168	2437.2	40.868
375.00	35.439	6.979	42.418	7.231	2617.2	40.955
400.00	35.890	6.997	42.887	7.297	2798.8	41.061
425.00	36.314	7.017	43.331	7.366	2982.0	41.182
450.00	36.716	7.038	43.754	7.435	3167.1	41.313
475.00	37.097	7.061	44.158	7.505	3353.8	41.452
500.00	37.460	7.085	44.545	7.572	3542.3	41.597
550.00	38.138	7.135	45.272	7.703	3924.2	41.899
600.00	38.761	7.187	45.948	7.823	4312.4	42.208
650.00	39.338	7.241	46.579	7.933	4706.4	42.520
700.00	39.876	7.294	47.170	8.032	5105.5	42.832
750.00	40.381	7.346	47.727	8.121	5509.4	43.140
800.00	40.857	7.397	48.254	8.201	5917.5	43.443
850.00	41.307	7.446	48.753	8.272	6329.4	43.741
900.00	41.734	7.494	49.228	8.336	6744.6	44.033
950.00	42.141	7.540	49.680	8.394	7162.9	44.318
1000.00	42.528	7.584	50.112	8.445	7583.9	44.597
1050.00	42.899	7.626	50.526	8.492	8007.4	44.870
1100.00	43.255	7.666	50.922	8.535	8433.0	45.136
1150.00	43.597	7.705	51.302	8.573	8860.8	45.396
1200.00	43.926	7.742	51.667	8.609	9290.3	45.649
1250.00	44.242	7.777	52.020	8.641	9721.6	45.897
1300.00	44.548	7.811	52.359	8.671	10154.4	46.139
1350.00	44.843	7.843	52.687	8.699	10588.6	46.376
1400.00	45.129	7.874	53.004	8.724	11024.2	46.607
1450.00	45.406	7.904	53.310	8.748	11461.0	46.833
1500.00	45.674	7.933	53.607	8.771	11899.0	47.054
1550.00	45.935	7.960	53.895	8.792	12338.1	47.270
1600.00	46.188	7.986	54.175	8.812	12778.2	47.481
1650.00	46.434	8.012	54.446	8.831	13219.2	47.688
1700.00	46.674	8.036	54.710	8.849	13661.2	47.891
1750.00	46.907	8.059	54.967	8.866	14104.1	48.089
1800.00	47.135	8.082	55.217	8.882	14547.8	48.284
1850.00	47.356	8.104	55.460	8.897	14992.2	48.474
1900.00	47.573	8.125	55.698	8.912	15437.5	48.661
1950.00	47.784	8.145	55.929	8.926	15883.5	48.845
2000.00	47.990	8.165	56.155	8.940	16330.1	49.025
2050.00	48.192	8.184	56.376	8.953	16777.4	49.201

Table A-91. Thermodynamic Functions for LiH(gas)-Continued

2100.00	48.390	8.203	56.592	8.965	17225.4	49.375
2150.00	48.583	8.220	56.803	8.977	17673.9	49.545
2200.00	48.772	8.238	57.010	8.988	18123.1	49.712
2250.00	48.957	8.255	57.212	8.999	18572.7	49.877
2300.00	49.139	8.271	57.410	9.008	19022.9	50.038
2350.00	49.317	8.287	57.604	9.018	19473.6	50.197
2400.00	49.492	8.302	57.794	9.026	19924.7	50.354
2450.00	49.663	8.317	57.980	9.034	20376.1	50.507
2500.00	49.831	8.331	58.162	9.041	20828.0	50.659
2600.00	50.159	8.359	58.517	9.052	21732.7	50.954
2700.00	50.474	8.385	58.859	9.060	22638.3	51.241
2800.00	50.780	8.409	59.189	9.064	23544.5	51.519
2900.00	51.075	8.431	59.507	9.064	24450.9	51.789
3000.00	51.361	8.452	59.814	9.060	25357.2	52.051
3100.00	51.639	8.472	60.111	9.052	26262.8	52.306
3200.00	51.908	8.490	60.398	9.039	27167.4	52.555
3300.00	52.170	8.506	60.676	9.022	28070.4	52.797
3400.00	52.424	8.521	60.945	9.000	28971.6	53.032
3500.00	52.671	8.534	61.205	8.975	29870.4	53.262
3600.00	52.912	8.546	61.458	8.945	30766.4	53.486
3700.00	53.146	8.557	61.703	8.911	31659.2	53.705
3800.00	53.374	8.565	61.940	8.874	32548.5	53.919
3900.00	53.597	8.573	62.170	8.833	33433.9	54.127
4000.00	53.814	8.579	62.393	8.789	34315.0	54.331
4100.00	54.026	8.583	62.609	8.742	35191.6	54.530
4200.00	54.233	8.587	62.819	8.693	36063.4	54.725
4300.00	54.435	8.588	63.023	8.641	36930.0	54.916
4400.00	54.632	8.589	63.221	8.587	37791.5	55.102
4500.00	54.825	8.588	63.414	8.531	38647.4	55.285
4600.00	55.014	8.586	63.600	8.474	39497.7	55.464
4700.00	55.199	8.583	63.782	8.416	40342.2	55.639
4800.00	55.379	8.579	63.959	8.356	41180.8	55.810
4900.00	55.556	8.574	64.130	8.296	42013.4	55.978
5000.00	55.729	8.568	64.297	8.235	42840.0	56.143
5100.00	55.899	8.561	64.460	8.174	43660.5	56.305
5200.00	56.065	8.553	64.618	8.113	44474.9	56.463
5300.00	56.228	8.544	64.772	8.052	45283.1	56.618
5400.00	56.388	8.534	64.922	7.991	46085.2	56.771
5500.00	56.544	8.524	65.068	7.930	46881.3	56.920
5600.00	56.698	8.513	65.210	7.870	47671.3	57.067
5700.00	56.848	8.501	65.349	7.810	48455.3	57.211
5800.00	56.996	8.489	65.484	7.751	49233.3	57.353
5900.00	57.141	8.476	65.616	7.692	50005.5	57.491
6000.00	57.283	8.462	65.745	7.635	50771.8	57.628

This table was computed for the ground electronic state ($^1\Sigma$) using a molecular weight of 7.94697 and the following molecular constants (in cm^{-1}): $\omega_e = 1405.649$, $x_e\omega_e = 23.2$, $y_e\omega_e = 0.1633$, $B_e = 7.5131$, $\alpha_e = 0.2132$, $\beta_e = 1.59(10^{-5})$, $\gamma_e = 7.5(10^{-4})$, $D_e = 8.617(10^{-4})$, D_0 (dissociation energy) = 57,600.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-92. Thermodynamic Functions for BeH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	34.690	6.913	41.603	6.948	1888.3	42.239
298.15	35.295	6.916	42.212	6.953	2062.1	42.212
50.00	23.045	6.758	29.803	6.954	337.9	64.287
75.00	25.799	6.823	32.622	6.952	511.7	53.294
100.00	27.767	6.855	34.622	6.950	685.5	48.388
125.00	29.299	6.874	36.173	6.949	859.2	45.795
150.00	30.553	6.886	37.440	6.948	1032.9	44.300
175.00	31.616	6.895	38.511	6.946	1206.6	43.399
200.00	32.537	6.901	39.438	6.945	1380.3	42.847
225.00	33.350	6.906	40.256	6.945	1553.9	42.515
250.00	34.078	6.910	40.988	6.945	1727.5	42.326
275.00	34.736	6.913	41.650	6.948	1901.2	42.235
300.00	35.338	6.916	42.255	6.953	2074.9	42.212
325.00	35.892	6.920	42.811	6.963	2248.9	42.237
350.00	36.405	6.923	43.328	6.976	2423.1	42.296
375.00	36.883	6.927	43.810	6.995	2597.7	42.381
400.00	37.330	6.932	44.262	7.018	2772.9	42.485
425.00	37.750	6.938	44.688	7.045	2948.7	42.602
450.00	38.147	6.945	45.092	7.077	3125.2	42.729
475.00	38.523	6.953	45.475	7.113	3302.6	42.864
500.00	38.880	6.962	45.841	7.153	3480.9	43.004
550.00	39.544	6.983	46.527	7.239	3840.6	43.293
600.00	40.153	7.008	47.161	7.331	4204.9	43.589
650.00	40.715	7.037	47.751	7.427	4573.8	43.887
700.00	41.237	7.068	48.305	7.522	4947.5	44.183
750.00	41.726	7.101	48.827	7.615	5326.0	44.476
800.00	42.186	7.136	49.322	7.705	5709.0	44.763
850.00	42.619	7.172	49.791	7.790	6096.4	45.045
900.00	43.030	7.209	50.239	7.870	6487.9	45.321
950.00	43.421	7.246	50.667	7.945	6883.3	45.592
1000.00	43.794	7.282	51.076	8.015	7282.3	45.856
1050.00	44.150	7.319	51.469	8.080	7684.8	46.114
1100.00	44.491	7.355	51.846	8.141	8090.3	46.366
1150.00	44.819	7.390	52.209	8.198	8498.8	46.612
1200.00	45.134	7.425	52.559	8.250	8910.0	46.852
1250.00	45.438	7.459	52.897	8.299	9323.7	47.087
1300.00	45.731	7.492	53.223	8.344	9739.8	47.317
1350.00	46.014	7.525	53.539	8.387	10158.1	47.542
1400.00	46.289	7.556	53.845	8.426	10578.5	47.762
1450.00	46.554	7.587	54.141	8.464	11000.7	47.976
1500.00	46.812	7.617	54.429	8.498	11424.8	48.187
1550.00	47.062	7.645	54.708	8.531	11850.5	48.393
1600.00	47.305	7.674	54.979	8.561	12277.8	48.594
1650.00	47.542	7.701	55.243	8.590	12706.6	48.792
1700.00	47.772	7.728	55.500	8.617	13136.8	48.985
1750.00	47.997	7.753	55.750	8.643	13568.4	49.175
1800.00	48.215	7.778	55.994	8.667	14001.1	49.361
1850.00	48.429	7.803	56.232	8.690	14435.1	49.543
1900.00	48.637	7.826	56.464	8.711	14870.1	49.723
1950.00	48.841	7.849	56.690	8.731	15306.2	49.898
2000.00	49.040	7.872	56.911	8.750	15743.2	50.071
2050.00	49.234	7.893	57.128	8.768	16181.2	50.240

Table A-92. Thermodynamic Functions for BeH(gas)-Continued

2100.00	49.425	7.914	57.339	8.784	16620.0	50.407
2150.00	49.611	7.935	57.546	8.799	17059.6	50.571
2200.00	49.794	7.955	57.749	8.813	17499.9	50.731
2250.00	49.973	7.974	57.947	8.826	17940.9	50.890
2300.00	50.148	7.992	58.141	8.838	18382.5	51.045
2350.00	50.321	8.010	58.331	8.848	18824.6	51.198
2400.00	50.489	8.028	58.517	8.857	19267.3	51.349
2450.00	50.655	8.045	58.700	8.864	19710.3	51.497
2500.00	50.818	8.061	58.879	8.870	20153.6	51.643
2600.00	51.135	8.093	59.227	8.879	21041.1	51.928
2700.00	51.441	8.122	59.562	8.881	21929.2	52.204
2800.00	51.736	8.149	59.885	8.879	22817.2	52.473
2900.00	52.023	8.174	60.197	8.870	23704.7	52.734
3000.00	52.300	8.197	60.497	8.856	24591.1	52.988
3100.00	52.569	8.218	60.787	8.837	25475.7	53.235
3200.00	52.831	8.237	61.068	8.812	26358.2	53.475
3300.00	53.084	8.254	61.338	8.782	27238.0	53.709
3400.00	53.331	8.269	61.600	8.748	28114.5	53.938
3500.00	53.571	8.282	61.853	8.709	28987.4	54.160
3600.00	53.804	8.293	62.098	8.666	29856.2	54.377
3700.00	54.032	8.303	62.335	8.620	30720.5	54.589
3800.00	54.253	8.311	62.564	8.570	31580.0	54.796
3900.00	54.469	8.317	62.786	8.517	32434.4	54.998
4000.00	54.680	8.321	63.001	8.462	33283.4	55.195
4100.00	54.885	8.324	63.209	8.404	34126.7	55.388
4200.00	55.086	8.325	63.411	8.345	34964.2	55.577
4300.00	55.282	8.325	63.606	8.284	35795.7	55.761
4400.00	55.473	8.323	63.796	8.223	36621.1	55.942
4500.00	55.660	8.320	63.980	8.160	37440.2	56.118
4600.00	55.843	8.316	64.159	8.096	38253.0	56.291
4700.00	56.022	8.311	64.332	8.033	39059.4	56.461
4800.00	56.197	8.304	64.501	7.969	39859.5	56.626
4900.00	56.368	8.297	64.664	7.905	40653.2	56.789
5000.00	56.535	8.288	64.824	7.841	41440.5	56.948
5100.00	56.699	8.279	64.978	7.778	42221.5	57.104
5200.00	56.860	8.268	65.129	7.716	42996.2	57.257
5300.00	57.018	8.257	65.275	7.654	43764.7	57.407
5400.00	57.172	8.246	65.417	7.593	44527.0	57.554
5500.00	57.323	8.233	65.556	7.532	45283.2	57.698
5600.00	57.471	8.220	65.691	7.473	46033.5	57.839
5700.00	57.617	8.207	65.823	7.415	46777.9	57.978
5800.00	57.759	8.193	65.952	7.358	47516.5	58.115
5900.00	57.899	8.178	66.077	7.302	48249.5	58.249
6000.00	58.036	8.163	66.199	7.247	48976.9	58.380

This table was computed for the ground electronic state ($^2\Sigma$) using a molecular weight of 10.02017 and the following molecular constants: $\omega_e = 2058.6$, $x_e\omega_e = 35.5$, $y_e\omega_e = -0.5$, $B_e = 10.308$, $\alpha_e = 0.3$, $D_e = 9.8(10^{-4})$, D_0 (dissociation energy) = 17,700.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-93. Thermodynamic Functions for NH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	35.780	6.893	42.673	6.946	1882.9	43.309
298.15	36.384	6.898	43.281	6.945	2056.5	43.281
50.00	24.231	6.638	30.870	6.953	331.9	65.361
75.00	26.946	6.743	33.689	6.954	505.8	54.366
100.00	28.894	6.796	35.689	6.953	679.6	49.459
125.00	30.414	6.827	37.241	6.952	853.4	46.866
150.00	31.660	6.848	38.508	6.951	1027.2	45.370
175.00	32.717	6.862	39.580	6.950	1200.9	44.469
200.00	33.634	6.873	40.507	6.949	1374.7	43.917
225.00	34.444	6.882	41.326	6.948	1548.4	43.584
250.00	35.170	6.888	42.058	6.947	1722.0	43.396
275.00	35.826	6.894	42.720	6.946	1895.7	43.305
300.00	36.426	6.898	43.324	6.945	2069.4	43.281
325.00	36.979	6.901	43.880	6.945	2243.0	43.306
350.00	37.490	6.905	44.395	6.944	2416.6	43.366
375.00	37.967	6.907	44.874	6.945	2590.2	43.451
400.00	38.413	6.910	45.322	6.945	2763.8	43.554
425.00	38.832	6.912	45.743	6.947	2937.5	43.670
450.00	39.227	6.914	46.140	6.950	3111.2	43.797
475.00	39.601	6.916	46.516	6.954	3285.0	43.930
500.00	39.955	6.918	46.873	6.959	3458.9	44.068
550.00	40.615	6.922	47.537	6.976	3807.2	44.354
600.00	41.217	6.928	48.145	7.000	4156.6	44.645
650.00	41.772	6.934	48.707	7.032	4507.4	44.936
700.00	42.286	6.943	49.229	7.071	4859.9	45.224
750.00	42.766	6.953	49.718	7.117	5214.6	45.508
800.00	43.215	6.965	50.179	7.168	5571.7	45.785
850.00	43.637	6.978	50.616	7.224	5931.5	46.057
900.00	44.037	6.993	51.030	7.282	6294.1	46.322
950.00	44.415	7.010	51.425	7.343	6659.8	46.580
1000.00	44.775	7.028	51.804	7.404	7028.4	46.832
1050.00	45.119	7.048	52.166	7.466	7400.2	47.077
1100.00	45.447	7.068	52.515	7.528	7775.0	47.317
1150.00	45.762	7.090	52.851	7.588	8152.9	47.550
1200.00	46.064	7.112	53.175	7.648	8533.8	47.778
1250.00	46.355	7.134	53.489	7.706	8917.7	48.000
1300.00	46.635	7.157	53.792	7.762	9304.4	48.217
1350.00	46.905	7.181	54.086	7.817	9693.9	48.429
1400.00	47.167	7.204	54.371	7.869	10086.0	48.636
1450.00	47.420	7.228	54.648	7.919	10480.7	48.838
1500.00	47.666	7.252	54.918	7.968	10877.9	49.037
1550.00	47.904	7.276	55.180	8.014	11277.5	49.231
1600.00	48.135	7.300	55.435	8.059	11679.3	49.420
1650.00	48.360	7.323	55.683	8.101	12083.3	49.607
1700.00	48.579	7.347	55.926	8.142	12489.4	49.789
1750.00	48.792	7.370	56.162	8.181	12897.5	49.968
1800.00	49.000	7.393	56.393	8.219	13307.5	50.143
1850.00	49.203	7.416	56.619	8.255	13719.4	50.315
1900.00	49.401	7.438	56.840	8.289	14133.0	50.484
1950.00	49.595	7.461	57.055	8.322	14548.2	50.649
2000.00	49.784	7.483	57.267	8.353	14965.1	50.812
2050.00	49.969	7.504	57.473	8.383	15383.5	50.972

Table A-93. Thermodynamic Functions for NH(gas)-Continued

2100.00	50.150	7.525	57.676	8.412	15803.4	51.129
2150.00	50.327	7.546	57.874	8.440	16224.7	51.284
2200.00	50.501	7.567	58.068	8.467	16647.4	51.436
2250.00	50.671	7.587	58.259	8.493	17071.5	51.585
2300.00	50.838	7.607	58.446	8.518	17496.7	51.733
2350.00	51.002	7.627	58.629	8.542	17923.2	51.877
2400.00	51.163	7.646	58.809	8.565	18350.9	52.020
2450.00	51.321	7.665	58.986	8.588	18779.7	52.160
2500.00	51.476	7.684	59.160	8.609	19209.7	52.299
2600.00	51.778	7.720	59.498	8.651	20072.7	52.569
2700.00	52.070	7.755	59.825	8.690	20939.7	52.832
2800.00	52.353	7.789	60.142	8.726	21810.5	53.087
2900.00	52.627	7.822	60.449	8.761	22684.9	53.336
3000.00	52.892	7.854	60.747	8.794	23562.7	53.578
3100.00	53.150	7.885	61.035	8.826	24443.7	53.814
3200.00	53.401	7.915	61.316	8.856	25327.8	54.044
3300.00	53.645	7.944	61.589	8.885	26214.8	54.268
3400.00	53.883	7.972	61.855	8.912	27104.7	54.488
3500.00	54.114	7.999	62.113	8.938	27997.2	54.702
3600.00	54.340	8.026	62.366	8.962	28892.1	54.911
3700.00	54.560	8.051	62.611	8.985	29789.5	55.116
3800.00	54.775	8.076	62.851	9.007	30689.1	55.316
3900.00	54.985	8.100	63.086	9.027	31590.8	55.513
4000.00	55.191	8.124	63.314	9.045	32494.4	55.705
4100.00	55.392	8.146	63.538	9.062	33399.7	55.893
4200.00	55.588	8.168	63.756	9.077	34306.7	56.078
4300.00	55.781	8.190	63.970	9.090	35215.0	56.259
4400.00	55.969	8.210	64.179	9.101	36124.6	56.437
4500.00	56.154	8.230	64.384	9.110	37035.2	56.611
4600.00	56.335	8.249	64.584	9.118	37946.6	56.782
4700.00	56.513	8.268	64.780	9.123	38858.6	56.950
4800.00	56.687	8.286	64.972	9.126	39771.0	57.115
4900.00	56.858	8.303	65.161	9.126	40683.6	57.278
5000.00	57.026	8.319	65.345	9.125	41596.2	57.437
5100.00	57.191	8.335	65.526	9.122	42508.6	57.594
5200.00	57.353	8.350	65.703	9.116	43420.5	57.748
5300.00	57.512	8.364	65.876	9.108	44331.7	57.900
5400.00	57.668	8.378	66.046	9.098	45242.0	58.049
5500.00	57.822	8.391	66.213	9.086	46151.3	58.196
5600.00	57.973	8.403	66.377	9.072	47059.2	58.341
5700.00	58.122	8.415	66.537	9.056	47965.6	58.483
5800.00	58.269	8.426	66.695	9.038	48870.2	58.623
5900.00	58.413	8.436	66.849	9.018	49773.0	58.761
6000.00	58.555	8.446	67.000	8.996	50673.7	58.897

This table was computed for the ground electronic state ($^3\Sigma^-$) using a molecular weight of 15.01467 and the following molecular constants (in cm^{-1}): $\omega_e = 3282.2$, $x_e\omega_e = 78.3$, $B_e = 16.668$, $\alpha_e = 0.646$, $\beta_e = 2(10^{-5})$, $D_e = 1.67(10^{-3})$, D_0 (dissociation energy) = 30,650.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-94. Thermodynamic Functions for NaH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	37.375	6.959	44.334	7.122	1900.9	44.989
298.15	37.985	6.976	44.961	7.194	2079.8	44.961
50.00	25.644	6.860	32.504	6.952	343.0	67.240
75.00	28.432	6.890	35.322	6.950	516.8	56.163
100.00	30.416	6.905	37.321	6.948	690.5	51.215
125.00	31.958	6.913	38.872	6.946	864.2	48.597
150.00	33.219	6.919	40.138	6.948	1037.8	47.085
175.00	34.286	6.924	41.210	6.958	1211.7	46.171
200.00	35.211	6.929	42.140	6.979	1385.8	45.610
225.00	36.028	6.937	42.964	7.015	1560.7	45.271
250.00	36.759	6.947	43.706	7.065	1736.7	45.078
275.00	37.422	6.960	44.382	7.127	1914.1	44.985
300.00	38.028	6.977	45.005	7.199	2093.1	44.961
325.00	38.587	6.997	45.584	7.278	2274.1	44.987
350.00	39.107	7.020	46.127	7.360	2457.1	45.049
375.00	39.592	7.046	46.637	7.444	2642.1	45.138
400.00	40.047	7.073	47.120	7.527	2829.3	45.247
425.00	40.477	7.102	47.579	7.609	3018.5	45.371
450.00	40.884	7.133	48.016	7.688	3209.7	45.506
475.00	41.270	7.164	48.434	7.763	3402.8	45.649
500.00	41.639	7.196	48.834	7.835	3597.8	45.798
550.00	42.327	7.260	49.587	7.967	3992.9	46.109
600.00	42.962	7.324	50.286	8.084	4394.3	46.428
650.00	43.550	7.386	50.937	8.186	4801.1	46.750
700.00	44.100	7.447	51.547	8.276	5212.7	47.071
750.00	44.616	7.505	52.120	8.355	5628.5	47.389
800.00	45.102	7.560	52.662	8.425	6048.0	47.702
850.00	45.562	7.613	53.175	8.486	6470.8	48.009
900.00	45.998	7.663	53.661	8.541	6896.5	48.309
950.00	46.414	7.710	54.124	8.591	7324.8	48.603
1000.00	46.811	7.756	54.566	8.635	7755.5	48.890
1050.00	47.190	7.798	54.989	8.676	8188.3	49.171
1100.00	47.554	7.839	55.393	8.713	8623.0	49.445
1150.00	47.903	7.878	55.781	8.747	9059.5	49.712
1200.00	48.239	7.915	56.154	8.778	9497.6	49.972
1250.00	48.563	7.950	56.513	8.808	9937.3	50.227
1300.00	48.876	7.983	56.859	8.835	10378.4	50.475
1350.00	49.177	8.015	57.193	8.861	10820.8	50.718
1400.00	49.469	8.046	57.516	8.886	11264.5	50.955
1450.00	49.752	8.075	57.828	8.910	11709.4	51.187
1500.00	50.027	8.104	58.130	8.933	12155.5	51.413
1550.00	50.293	8.131	58.424	8.955	12602.7	51.635
1600.00	50.551	8.157	58.708	8.977	13051.0	51.851
1650.00	50.803	8.182	58.985	8.998	13500.4	52.063
1700.00	51.047	8.206	59.254	9.019	13950.9	52.271
1750.00	51.286	8.230	59.515	9.039	14402.3	52.474
1800.00	51.518	8.253	59.770	9.059	14854.8	52.673
1850.00	51.744	8.275	60.019	9.079	15308.3	52.868
1900.00	51.965	8.296	60.261	9.099	15762.7	53.060
1950.00	52.181	8.317	60.498	9.118	16218.1	53.247
2000.00	52.392	8.337	60.729	9.136	16674.5	53.432
2050.00	52.598	8.357	60.955	9.154	17131.7	53.612

Table A-94. Thermodynamic Functions for NaH(gas)-Continued

2100.00	52.799	8.376	61.176	9.172	17589.9	53.790
2150.00	52.997	8.395	61.392	9.189	18048.9	53.964
2200.00	53.190	8.413	61.603	9.206	18508.8	54.135
2250.00	53.379	8.431	61.810	9.221	18969.5	54.304
2300.00	53.565	8.448	62.013	9.236	19430.9	54.469
2350.00	53.747	8.465	62.212	9.250	19893.1	54.632
2400.00	53.925	8.482	62.407	9.263	20355.9	54.792
2450.00	54.100	8.498	62.598	9.275	20819.4	54.949
2500.00	54.272	8.513	62.785	9.286	21283.5	55.104
2600.00	54.606	8.543	63.150	9.304	22213.0	55.406
2700.00	54.929	8.572	63.501	9.316	23144.0	55.700
2800.00	55.242	8.599	63.840	9.322	24075.9	55.984
2900.00	55.544	8.623	64.167	9.321	25008.1	56.261
3000.00	55.836	8.647	64.483	9.314	25939.9	56.530
3100.00	56.120	8.668	64.788	9.300	26870.6	56.791
3200.00	56.396	8.687	65.083	9.279	27799.6	57.046
3300.00	56.663	8.705	65.368	9.251	28726.1	57.294
3400.00	56.924	8.720	65.644	9.218	29649.7	57.535
3500.00	57.176	8.734	65.911	9.178	30569.5	57.771
3600.00	57.423	8.746	66.169	9.133	31485.1	58.000
3700.00	57.662	8.756	66.418	9.082	32395.9	58.225
3800.00	57.896	8.764	66.660	9.027	33301.4	58.443
3900.00	58.124	8.770	66.893	8.968	34201.2	58.657
4000.00	58.346	8.774	67.120	8.905	35094.9	58.866
4100.00	58.563	8.776	67.339	8.839	35982.1	59.070
4200.00	58.774	8.777	67.551	8.770	36862.6	59.269
4300.00	58.981	8.776	67.756	8.699	37736.1	59.464
4400.00	59.182	8.773	67.956	8.627	38602.4	59.655
4500.00	59.379	8.769	68.149	8.553	39461.4	59.842
4600.00	59.572	8.764	68.336	8.478	40312.9	60.024
4700.00	59.760	8.757	68.517	8.402	41156.9	60.203
4800.00	59.945	8.749	68.693	8.326	41993.3	60.378
4900.00	60.125	8.739	68.864	8.250	42822.1	60.550
5000.00	60.302	8.729	69.030	8.174	43643.3	60.717
5100.00	60.474	8.717	69.191	8.099	44457.0	60.882
5200.00	60.643	8.704	69.348	8.025	45263.2	61.043
5300.00	60.809	8.691	69.500	7.951	46062.0	61.201
5400.00	60.971	8.677	69.648	7.878	46853.4	61.357
5500.00	61.130	8.661	69.792	7.806	47637.6	61.509
5600.00	61.286	8.645	69.932	7.736	48414.7	61.658
5700.00	61.439	8.629	70.068	7.667	49184.9	61.804
5800.00	61.589	8.612	70.201	7.599	49948.2	61.948
5900.00	61.736	8.594	70.330	7.533	50704.8	62.089
6000.00	61.881	8.576	70.456	7.468	51454.8	62.227

This table was computed for the ground electronic state ($^1\Sigma$) using a molecular weight of 23.99777 and the following molecular constants (in cm^{-1}): $\omega_e = 1172.2$, $x_e\omega_e = 19.72$, $y_e\omega_e = 0.160$, $z_e\omega_e = -0.005$, $B_e = 4.9012$, $\alpha_e = 0.1353$, $\beta_e = 3(10^{-6})$, $D_e = 3.32(10^{-4})$, D_0 (dissociation energy) = 50,600.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-95. Thermodynamic Functions for PH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	39.348	6.921	46.269	6.948	1890.6	46.905
298.15	39.954	6.924	46.878	6.949	2064.3	46.878
50.00	27.672	6.794	34.466	6.954	339.7	68.958
75.00	30.438	6.847	37.286	6.953	513.5	57.962
100.00	32.412	6.874	39.286	6.952	687.4	53.055
125.00	33.948	6.889	40.837	6.951	861.1	50.462
150.00	35.205	6.899	42.104	6.950	1034.9	48.967
175.00	36.269	6.907	43.176	6.949	1208.7	48.065
200.00	37.192	6.912	44.103	6.948	1382.4	47.513
225.00	38.006	6.916	44.922	6.948	1556.1	47.181
250.00	38.735	6.919	45.654	6.947	1729.8	46.992
275.00	39.394	6.922	46.316	6.948	1903.5	46.901
300.00	39.997	6.924	46.920	6.949	2077.2	46.878
325.00	40.551	6.926	47.477	6.952	2250.9	46.903
350.00	41.064	6.928	47.992	6.957	2424.8	46.962
375.00	41.542	6.930	48.472	6.965	2598.8	47.047
400.00	41.990	6.933	48.922	6.976	2773.1	47.150
425.00	42.410	6.936	49.346	6.991	2947.6	47.267
450.00	42.807	6.939	49.746	7.009	3122.6	47.394
475.00	43.182	6.943	50.125	7.031	3298.1	47.528
500.00	43.538	6.948	50.486	7.055	3474.2	47.667
550.00	44.201	6.961	51.162	7.114	3828.4	47.954
600.00	44.807	6.976	51.784	7.183	4185.8	48.248
650.00	45.366	6.995	52.361	7.258	4546.8	48.542
700.00	45.886	7.017	52.902	7.338	4911.7	48.835
750.00	46.370	7.041	53.411	7.420	5280.6	49.123
800.00	46.826	7.067	53.893	7.501	5653.6	49.406
850.00	47.255	7.095	54.350	7.581	6030.7	49.684
900.00	47.661	7.124	54.785	7.659	6411.8	49.955
950.00	48.047	7.154	55.202	7.734	6796.6	50.220
1000.00	48.415	7.185	55.600	7.805	7185.1	50.479
1050.00	48.766	7.216	55.983	7.872	7577.0	50.732
1100.00	49.103	7.248	56.350	7.936	7972.3	50.979
1150.00	49.426	7.279	56.704	7.996	8370.6	51.221
1200.00	49.736	7.310	57.046	8.052	8771.8	51.456
1250.00	50.035	7.341	57.376	8.105	9175.8	51.687
1300.00	50.324	7.371	57.695	8.155	9582.3	51.911
1350.00	50.602	7.401	58.003	8.201	9991.2	52.131
1400.00	50.872	7.430	58.302	8.244	10402.3	52.346
1450.00	51.133	7.459	58.592	8.285	10815.5	52.557
1500.00	51.387	7.487	58.874	8.323	11230.8	52.763
1550.00	51.633	7.515	59.147	8.359	11647.8	52.964
1600.00	51.872	7.542	59.413	8.393	12066.6	53.162
1650.00	52.104	7.568	59.672	8.424	12487.0	53.355
1700.00	52.330	7.594	59.924	8.454	12909.0	53.545
1750.00	52.551	7.619	60.169	8.482	13332.4	53.730
1800.00	52.766	7.643	60.409	8.509	13757.2	53.913
1850.00	52.975	7.667	60.642	8.534	14183.2	54.091
1900.00	53.180	7.690	60.870	8.557	14610.5	54.267
1950.00	53.380	7.712	61.093	8.580	15038.9	54.439
2000.00	53.576	7.734	61.310	8.601	15468.5	54.608
2050.00	53.767	7.756	61.523	8.621	15899.0	54.774

Table A-95. Thermodynamic Functions for PH(gas)-Continued

2100.00	53.954	7.776	61.731	8.640	16330.5	54.937
2150.00	54.137	7.797	61.934	8.658	16763.0	55.098
2200.00	54.317	7.817	62.133	8.676	17196.3	55.255
2250.00	54.493	7.836	62.329	8.692	17630.5	55.410
2300.00	54.665	7.855	62.520	8.708	18065.5	55.563
2350.00	54.834	7.873	62.707	8.723	18501.3	55.713
2400.00	55.000	7.891	62.891	8.737	18937.8	55.860
2450.00	55.163	7.908	63.071	8.751	19375.0	56.006
2500.00	55.323	7.925	63.248	8.764	19812.9	56.149
2600.00	55.635	7.958	63.592	8.788	20690.4	56.429
2700.00	55.935	7.989	63.924	8.809	21570.3	56.700
2800.00	56.227	8.019	64.245	8.828	22452.2	56.964
2900.00	56.508	8.047	64.555	8.845	23335.8	57.220
3000.00	56.782	8.074	64.855	8.859	24221.1	57.470
3100.00	57.047	8.099	65.146	8.871	25107.6	57.713
3200.00	57.304	8.124	65.428	8.881	25995.2	57.949
3300.00	57.555	8.147	65.701	8.887	26883.7	58.180
3400.00	57.798	8.168	65.967	8.892	27772.6	58.405
3500.00	58.035	8.189	66.224	8.893	28661.9	58.625
3600.00	58.266	8.209	66.475	8.892	29551.2	58.840
3700.00	58.491	8.227	66.719	8.888	30440.2	59.049
3800.00	58.711	8.244	66.955	8.881	31328.6	59.254
3900.00	58.925	8.261	67.186	8.871	32216.2	59.455
4000.00	59.135	8.276	67.410	8.859	33102.8	59.651
4100.00	59.339	8.290	67.629	8.843	33987.9	59.843
4200.00	59.539	8.303	67.842	8.825	34871.3	60.031
4300.00	59.735	8.315	68.049	8.805	35752.9	60.215
4400.00	59.926	8.326	68.252	8.782	36632.2	60.395
4500.00	60.113	8.335	68.449	8.756	37509.1	60.572
4600.00	60.297	8.344	68.641	8.728	38383.3	60.745
4700.00	60.476	8.352	68.828	8.698	39254.7	60.915
4800.00	60.652	8.359	69.011	8.666	40122.9	61.082
4900.00	60.824	8.365	69.189	8.632	40987.8	61.246
5000.00	60.993	8.370	69.363	8.596	41849.2	61.406
5100.00	61.159	8.374	69.533	8.559	42707.0	61.564
5200.00	61.322	8.377	69.699	8.520	43560.9	61.719
5300.00	61.481	8.379	69.861	8.479	44410.9	61.871
5400.00	61.638	8.381	70.019	8.438	45256.8	62.020
5500.00	61.792	8.382	70.173	8.395	46098.4	62.167
5600.00	61.943	8.381	70.324	8.352	46935.8	62.312
5700.00	62.091	8.380	70.472	8.307	47768.8	62.453
5800.00	62.237	8.379	70.616	8.262	48597.3	62.593
5900.00	62.380	8.376	70.757	8.217	49421.2	62.730
6000.00	62.521	8.373	70.894	8.171	50240.6	62.865

This table was computed for the ground electronic state ($^3\Sigma^-$) using a molecular weight of 31.98177 and the following molecular constants (in cm^{-1}): $\omega_e = 2380$, $x_e\omega_e = 35$, $B_e = 8.4120$, $\alpha_e = 0.185$, $D_e = 4.3(10^{-4})$, D_0 (dissociation energy) = 24,200.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-96. Thermodynamic Functions for KH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	39.624	7.000	46.624	7.276	1912.1	47.294
298.15	40.238	7.027	47.265	7.373	2095.2	47.265
50.00	27.862	6.889	34.750	6.952	344.4	69.766
75.00	30.659	6.909	37.569	6.950	518.2	58.596
100.00	32.649	6.919	39.568	6.948	691.9	53.601
125.00	34.193	6.925	41.118	6.950	865.6	50.955
150.00	35.456	6.930	42.386	6.962	1039.5	49.424
175.00	36.525	6.936	43.461	6.991	1213.9	48.498
200.00	37.452	6.946	44.398	7.040	1389.2	47.928
225.00	38.271	6.960	45.231	7.108	1566.0	47.583
250.00	39.005	6.979	45.984	7.190	1744.7	47.386
275.00	39.671	7.002	46.673	7.283	1925.6	47.290
300.00	40.281	7.030	47.311	7.380	2108.9	47.265
325.00	40.845	7.060	47.906	7.479	2294.6	47.292
350.00	41.370	7.094	48.463	7.576	2482.8	47.356
375.00	41.860	7.129	48.989	7.670	2673.4	47.448
400.00	42.322	7.166	49.487	7.759	2866.3	47.560
425.00	42.757	7.203	49.960	7.843	3061.3	47.687
450.00	43.170	7.241	50.411	7.922	3258.4	47.826
475.00	43.562	7.279	50.841	7.995	3457.3	47.973
500.00	43.937	7.316	51.253	8.063	3658.1	48.127
550.00	44.637	7.390	52.027	8.183	4064.3	48.447
600.00	45.283	7.460	52.744	8.287	4476.1	48.776
650.00	45.883	7.527	53.411	8.375	4892.7	49.107
700.00	46.443	7.591	54.034	8.451	5313.4	49.437
750.00	46.969	7.650	54.619	8.517	5737.7	49.763
800.00	47.465	7.706	55.171	8.575	6165.0	50.084
850.00	47.934	7.759	55.692	8.625	6595.0	50.398
900.00	48.378	7.808	56.187	8.670	7027.4	50.706
950.00	48.802	7.855	56.657	8.711	7462.0	51.007
1000.00	49.206	7.898	57.104	8.748	7898.4	51.301
1050.00	49.592	7.940	57.532	8.781	8336.7	51.588
1100.00	49.963	7.979	57.941	8.812	8776.5	51.867
1150.00	50.318	8.015	58.333	8.840	9217.8	52.140
1200.00	50.660	8.050	58.710	8.867	9660.5	52.406
1250.00	50.989	8.084	59.073	8.893	10104.5	52.665
1300.00	51.307	8.115	59.422	8.917	10549.8	52.919
1350.00	51.614	8.145	59.759	8.940	10996.2	53.166
1400.00	51.910	8.174	60.085	8.962	11443.7	53.407
1450.00	52.198	8.202	60.399	8.984	11892.4	53.643
1500.00	52.476	8.228	60.704	9.004	12342.1	53.873
1550.00	52.746	8.253	61.000	9.024	12792.8	54.098
1600.00	53.009	8.278	61.287	9.044	13244.5	54.318
1650.00	53.264	8.301	61.565	9.062	13697.2	54.534
1700.00	53.512	8.324	61.836	9.080	14150.7	54.745
1750.00	53.754	8.346	62.100	9.097	14605.1	54.951
1800.00	53.989	8.367	62.356	9.113	15060.4	55.153
1850.00	54.219	8.387	62.606	9.128	15516.4	55.351
1900.00	54.443	8.407	62.850	9.142	15973.2	55.545
1950.00	54.661	8.426	63.087	9.154	16430.6	55.736
2000.00	54.875	8.444	63.319	9.165	16888.6	55.922
2050.00	55.084	8.462	63.546	9.175	17347.1	56.106

Table A-96. Thermodynamic Functions for KH(gas)-Continued

2100.00	55.288	8.479	63.767	9.183	17806.1	56.285
2150.00	55.487	8.496	63.983	9.189	18265.4	56.462
2200.00	55.683	8.511	64.194	9.193	18724.9	56.635
2250.00	55.874	8.527	64.401	9.195	19184.6	56.805
2300.00	56.062	8.541	64.603	9.196	19644.4	56.973
2350.00	56.246	8.555	64.801	9.194	20104.2	57.137
2400.00	56.426	8.568	64.994	9.190	20563.8	57.299
2450.00	56.603	8.581	65.184	9.184	21023.2	57.458
2500.00	56.776	8.593	65.369	9.176	21482.2	57.614
2600.00	57.114	8.615	65.729	9.153	22398.7	57.920
2700.00	57.439	8.634	66.073	9.122	23312.5	58.215
2800.00	57.753	8.651	66.404	9.082	24222.8	58.502
2900.00	58.057	8.665	66.722	9.035	25128.7	58.780
3000.00	58.351	8.677	67.028	8.981	26029.6	59.050
3100.00	58.636	8.685	67.321	8.920	26924.7	59.312
3200.00	58.912	8.692	67.603	8.854	27813.5	59.567
3300.00	59.179	8.696	67.875	8.783	28695.4	59.814
3400.00	59.439	8.697	68.136	8.708	29570.0	60.055
3500.00	59.691	8.696	68.387	8.630	30436.9	60.290
3600.00	59.936	8.693	68.629	8.548	31295.8	60.518
3700.00	60.174	8.688	68.862	8.465	32146.5	60.740
3800.00	60.406	8.681	69.087	8.380	32988.8	60.957
3900.00	60.631	8.672	69.304	8.295	33822.5	61.168
4000.00	60.851	8.662	69.512	8.209	34647.7	61.374
4100.00	61.064	8.650	69.714	8.123	35464.3	61.575
4200.00	61.273	8.636	69.909	8.038	36272.4	61.771
4300.00	61.476	8.621	70.097	7.953	37071.9	61.963
4400.00	61.674	8.605	70.279	7.869	37863.0	62.150
4500.00	61.867	8.588	70.455	7.787	38645.8	62.332
4600.00	62.055	8.570	70.625	7.706	39420.4	62.511
4700.00	62.239	8.550	70.790	7.627	40187.1	62.685
4800.00	62.419	8.530	70.950	7.549	40945.9	62.856
4900.00	62.595	8.510	71.105	7.474	41697.0	63.023
5000.00	62.767	8.488	71.255	7.400	42440.7	63.186
5100.00	62.935	8.466	71.401	7.329	43177.2	63.345
5200.00	63.099	8.444	71.542	7.259	43906.5	63.502
5300.00	63.259	8.421	71.680	7.191	44629.0	63.655
5400.00	63.416	8.397	71.814	7.126	45344.9	63.805
5500.00	63.570	8.374	71.944	7.062	46054.3	63.951
5600.00	63.721	8.350	72.071	7.001	46757.4	64.095
5700.00	63.869	8.325	72.194	6.941	47454.5	64.236
5800.00	64.013	8.301	72.314	6.884	48145.8	64.374
5900.00	64.155	8.277	72.431	6.828	48831.4	64.510
6000.00	64.294	8.252	72.546	6.775	49511.5	64.643

This table was computed for the ground electronic state ($^1\Sigma$) using a molecular weight of 40.10997 and the following molecular constants (in cm^{-1}): $\omega_e = 985$, $x_e\omega_e = 14.65$, $B_e = 3.4070$, $\alpha_e = 0.0673$, $\gamma_e = -9.6(10^{-4})$, $D_e = 1.57(10^{-4})$, D_0 (dissociation energy) = 15,000.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm.

Table A-97. Thermodynamic Functions for CaH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	40.618	6.950	47.569	7.058	1898.5	48.217
298.15	41.227	6.962	48.189	7.112	2075.6	48.189
50.00	28.878	6.873	35.751	6.953	343.6	70.391
75.00	31.671	6.899	38.570	6.951	517.4	59.346
100.00	33.657	6.912	40.569	6.950	691.2	54.413
125.00	35.200	6.919	42.120	6.948	864.9	51.805
150.00	36.462	6.924	43.387	6.948	1038.6	50.300
175.00	37.530	6.928	44.458	6.952	1212.4	49.391
200.00	38.455	6.931	45.387	6.963	1386.3	48.833
225.00	39.272	6.936	46.208	6.985	1560.6	48.497
250.00	40.003	6.942	46.946	7.017	1735.6	48.306
275.00	40.665	6.951	47.616	7.062	1911.6	48.213
300.00	41.271	6.963	48.233	7.116	2088.8	48.189
325.00	41.828	6.977	48.805	7.179	2267.5	48.215
350.00	42.346	6.994	49.340	7.248	2447.8	48.276
375.00	42.829	7.013	49.842	7.320	2629.9	48.364
400.00	43.282	7.035	50.317	7.395	2813.8	48.472
425.00	43.710	7.058	50.768	7.470	2999.6	48.593
450.00	44.114	7.083	51.197	7.545	3187.3	48.726
475.00	44.497	7.109	51.607	7.618	3376.9	48.867
500.00	44.863	7.136	51.999	7.688	3568.2	49.014
550.00	45.546	7.193	52.738	7.821	3955.9	49.319
600.00	46.174	7.250	53.424	7.941	4350.0	49.633
650.00	46.756	7.307	54.064	8.048	4749.8	49.950
700.00	47.300	7.364	54.664	8.144	5154.7	50.265
750.00	47.810	7.419	55.229	8.229	5564.0	50.577
800.00	48.290	7.472	55.762	8.305	5977.4	50.885
850.00	48.745	7.523	56.268	8.372	6394.3	51.187
900.00	49.176	7.572	56.748	8.432	6814.5	51.483
950.00	49.587	7.618	57.205	8.486	7237.4	51.772
1000.00	49.979	7.663	57.642	8.534	7662.9	52.054
1050.00	50.354	7.705	58.059	8.578	8090.7	52.331
1100.00	50.713	7.746	58.459	8.617	8520.6	52.600
1150.00	51.058	7.785	58.843	8.653	8952.4	52.863
1200.00	51.390	7.822	59.212	8.686	9385.9	53.120
1250.00	51.710	7.857	59.567	8.717	9821.0	53.371
1300.00	52.019	7.890	59.910	8.745	10257.5	53.616
1350.00	52.318	7.923	60.240	8.770	10695.4	53.855
1400.00	52.606	7.953	60.560	8.794	11134.5	54.089
1450.00	52.886	7.983	60.869	8.815	11574.7	54.317
1500.00	53.157	8.011	61.168	8.835	12016.0	54.541
1550.00	53.420	8.038	61.458	8.852	12458.2	54.759
1600.00	53.676	8.063	61.739	8.868	12901.2	54.973
1650.00	53.924	8.088	62.012	8.882	13345.0	55.182
1700.00	54.166	8.111	62.277	8.894	13789.4	55.387
1750.00	54.402	8.134	62.535	8.904	14234.3	55.588
1800.00	54.631	8.155	62.786	8.912	14679.8	55.784
1850.00	54.855	8.176	63.031	8.918	15125.5	55.977
1900.00	55.073	8.196	63.269	8.921	15571.5	56.165
1950.00	55.286	8.214	63.500	8.923	16017.6	56.351
2000.00	55.494	8.232	63.726	8.922	16463.8	56.532
2050.00	55.698	8.249	63.946	8.919	16909.8	56.710

Table A-97. Thermodynamic Functions for CaH(gas)-Continued

2100.00	55.897	8.265	64.161	8.914	17355.6	56.885
2150.00	56.091	8.280	64.371	8.906	17801.1	57.057
2200.00	56.282	8.294	64.576	8.896	18246.2	57.225
2250.00	56.468	8.307	64.775	8.884	18690.7	57.391
2300.00	56.651	8.319	64.971	8.869	19134.6	57.554
2350.00	56.830	8.331	65.161	8.853	19577.6	57.713
2400.00	57.006	8.342	65.347	8.834	20019.8	57.871
2450.00	57.178	8.351	65.529	8.813	20461.0	58.025
2500.00	57.347	8.360	65.707	8.790	20901.1	58.177
2600.00	57.675	8.376	66.051	8.739	21777.6	58.473
2700.00	57.991	8.388	66.380	8.681	22648.6	58.760
2800.00	58.296	8.398	66.694	8.616	23513.5	59.038
2900.00	58.591	8.404	66.995	8.546	24371.7	59.307
3000.00	58.876	8.408	67.284	8.472	25222.6	59.568
3100.00	59.152	8.408	67.560	8.394	26066.0	59.821
3200.00	59.419	8.407	67.826	8.314	26901.4	60.067
3300.00	59.677	8.403	68.080	8.231	27728.7	60.306
3400.00	59.928	8.396	68.325	8.147	28547.6	60.539
3500.00	60.172	8.388	68.560	8.062	29358.1	60.765
3600.00	60.408	8.378	68.785	7.977	30160.1	60.984
3700.00	60.637	8.366	69.003	7.892	30953.5	61.198
3800.00	60.860	8.352	69.212	7.808	31738.5	61.406
3900.00	61.077	8.337	69.414	7.724	32515.1	61.609
4000.00	61.288	8.321	69.608	7.642	33283.4	61.807
4100.00	61.493	8.303	69.796	7.561	34043.5	61.999
4200.00	61.693	8.285	69.977	7.482	34795.7	62.187
4300.00	61.887	8.265	70.153	7.405	35540.0	62.370
4400.00	62.077	8.245	70.322	7.330	36276.7	62.549
4500.00	62.262	8.224	70.486	7.256	37006.0	62.724
4600.00	62.443	8.202	70.645	7.185	37728.0	62.894
4700.00	62.619	8.179	70.798	7.116	38443.1	63.061
4800.00	62.791	8.157	70.947	7.049	39151.3	63.223
4900.00	62.959	8.133	71.092	6.984	39853.0	63.382
5000.00	63.123	8.110	71.233	6.922	40548.2	63.538
5100.00	63.283	8.086	71.369	6.861	41237.4	63.690
5200.00	63.440	8.062	71.502	6.803	41920.6	63.839
5300.00	63.593	8.037	71.631	6.746	42598.0	63.985
5400.00	63.743	8.013	71.756	6.692	43269.9	64.128
5500.00	63.890	7.988	71.879	6.640	43936.5	64.268
5600.00	64.034	7.964	71.998	6.589	44597.9	64.405
5700.00	64.175	7.939	72.114	6.540	45254.4	64.539
5800.00	64.313	7.915	72.227	6.494	45906.1	64.670
5900.00	64.448	7.890	72.338	6.448	46553.1	64.799
6000.00	64.580	7.866	72.446	6.405	47195.8	64.926

This table was computed for the ground electronic state ($^2\Sigma$) using a molecular weight of 41.08797 and the following molecular constants (in cm^{-1}): $\omega_e = 1299$, $x_e\omega_e = 19.5$, $B_e = 4.2778$, $\alpha_e = 0.0963$, $\beta_e = 2(10^{-6})$, $D_e = 1.84(10^{-4})$, D_0 (dissociation energy) = 13,500.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-98. Thermodynamic Functions for SrH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/
273.15	43.211	6.961	50.172	7.103	1901.5	50.825
298.15	43.821	6.976	50.797	7.168	2079.8	50.797
50.00	31.460	6.884	38.344	6.953	344.2	73.056
75.00	34.256	6.907	41.162	6.951	518.0	61.987
100.00	36.244	6.918	43.162	6.950	691.8	57.043
125.00	37.789	6.924	44.713	6.949	865.5	54.427
150.00	39.052	6.928	45.980	6.950	1039.2	52.917
175.00	40.120	6.932	47.052	6.958	1213.1	52.004
200.00	41.046	6.936	47.982	6.976	1387.2	51.445
225.00	41.863	6.942	48.805	7.007	1562.0	51.107
250.00	42.595	6.951	49.545	7.051	1737.6	50.914
275.00	43.258	6.962	50.220	7.107	1914.6	50.821
300.00	43.864	6.977	50.841	7.174	2093.1	50.797
325.00	44.423	6.995	51.418	7.247	2273.3	50.823
350.00	44.942	7.016	51.958	7.326	2455.5	50.885
375.00	45.427	7.039	52.466	7.406	2639.6	50.973
400.00	45.882	7.065	52.947	7.487	2825.8	51.082
425.00	46.311	7.092	53.403	7.567	3014.0	51.205
450.00	46.718	7.120	53.838	7.644	3204.1	51.339
475.00	47.103	7.150	54.253	7.719	3396.2	51.482
500.00	47.471	7.180	54.651	7.790	3590.0	51.630
550.00	48.158	7.242	55.400	7.922	3982.9	51.940
600.00	48.791	7.303	56.094	8.040	4382.0	52.257
650.00	49.378	7.364	56.742	8.143	4786.6	52.577
700.00	49.926	7.423	57.349	8.234	5196.1	52.897
750.00	50.440	7.480	57.920	8.315	5609.9	53.213
800.00	50.924	7.534	58.459	8.386	6027.4	53.524
850.00	51.383	7.586	58.969	8.448	6448.3	53.829
900.00	51.818	7.636	59.453	8.504	6872.1	54.129
950.00	52.232	7.683	59.914	8.554	7298.6	54.421
1000.00	52.627	7.727	60.354	8.599	7727.5	54.707
1050.00	53.005	7.770	60.775	8.639	8158.5	54.986
1100.00	53.367	7.810	61.178	8.676	8591.4	55.258
1150.00	53.715	7.849	61.564	8.710	9026.0	55.524
1200.00	54.050	7.885	61.936	8.741	9462.3	55.783
1250.00	54.373	7.920	62.293	8.769	9900.0	56.037
1300.00	54.684	7.953	62.637	8.795	10339.1	56.284
1350.00	54.985	7.985	62.970	8.819	10779.5	56.526
1400.00	55.276	8.015	63.291	8.841	11221.0	56.761
1450.00	55.558	8.044	63.601	8.861	11663.6	56.992
1500.00	55.831	8.071	63.902	8.880	12107.1	57.217
1550.00	56.096	8.098	64.194	8.897	12551.5	57.438
1600.00	56.353	8.123	64.476	8.912	12996.7	57.653
1650.00	56.604	8.147	64.751	8.925	13442.7	57.864
1700.00	56.847	8.170	65.017	8.936	13889.2	58.071
1750.00	57.084	8.192	65.277	8.946	14336.2	58.273
1800.00	57.315	8.213	65.529	8.953	14783.7	58.471
1850.00	57.541	8.233	65.774	8.958	15231.5	58.665
1900.00	57.761	8.252	66.013	8.961	15679.5	58.855
1950.00	57.975	8.271	66.246	8.962	16127.6	59.042
2000.00	58.185	8.288	66.473	8.961	16575.7	59.225
2050.00	58.390	8.304	66.694	8.958	17023.7	59.404

Table A-98. Thermodynamic Functions for SrH(gas)-Continued

2100.00	58.590	8.320	66.910	8.952	17471.4	59.580
2150.00	58.786	8.334	67.120	8.944	17918.8	59.753
2200.00	58.978	8.348	67.326	8.933	18365.8	59.923
2250.00	59.165	8.361	67.526	8.920	18812.1	60.090
2300.00	59.349	8.373	67.722	8.905	19257.7	60.254
2350.00	59.530	8.384	67.914	8.888	19702.6	60.415
2400.00	59.706	8.394	68.101	8.869	20146.5	60.573
2450.00	59.879	8.404	68.283	8.847	20589.4	60.728
2500.00	60.049	8.412	68.462	8.823	21031.2	60.881
2600.00	60.379	8.427	68.807	8.771	21910.9	61.179
2700.00	60.698	8.439	69.137	8.711	22785.1	61.468
2800.00	61.005	8.447	69.452	8.645	23652.9	61.748
2900.00	61.301	8.453	69.754	8.573	24513.8	62.018
3000.00	61.588	8.456	70.044	8.498	25367.4	62.281
3100.00	61.865	8.456	70.321	8.418	26213.2	62.536
3200.00	62.134	8.453	70.587	8.336	27051.0	62.784
3300.00	62.394	8.449	70.842	8.252	27880.4	63.024
3400.00	62.646	8.442	71.087	8.166	28701.3	63.258
3500.00	62.890	8.432	71.323	8.080	29513.6	63.485
3600.00	63.128	8.421	71.549	7.993	30317.2	63.706
3700.00	63.358	8.409	71.767	7.907	31112.2	63.920
3800.00	63.582	8.394	71.977	7.821	31898.6	64.130
3900.00	63.800	8.379	72.179	7.736	32676.4	64.334
4000.00	64.012	8.361	72.374	7.653	33445.9	64.532
4100.00	64.218	8.343	72.562	7.571	34207.1	64.726
4200.00	64.419	8.324	72.743	7.491	34960.1	64.914
4300.00	64.615	8.304	72.918	7.413	35705.3	65.099
4400.00	64.806	8.282	73.088	7.336	36442.7	65.278
4500.00	64.991	8.261	73.252	7.262	37172.7	65.454
4600.00	65.173	8.238	73.411	7.190	37895.3	65.625
4700.00	65.350	8.215	73.565	7.121	38610.8	65.792
4800.00	65.522	8.192	73.714	7.053	39319.5	65.956
4900.00	65.691	8.168	73.859	6.988	40021.5	66.115
5000.00	65.856	8.143	73.999	6.924	40717.1	66.272
5100.00	66.017	8.119	74.136	6.863	41406.4	66.425
5200.00	66.174	8.094	74.268	6.805	42089.8	66.574
5300.00	66.328	8.069	74.397	6.748	42767.4	66.721
5400.00	66.479	8.044	74.523	6.693	43439.4	66.864
5500.00	66.626	8.019	74.645	6.640	44106.0	67.004
5600.00	66.770	7.994	74.765	6.589	44767.5	67.142
5700.00	66.912	7.969	74.881	6.540	45424.0	67.277
5800.00	67.050	7.944	74.994	6.493	46075.6	67.409
5900.00	67.186	7.919	75.105	6.448	46722.6	67.538
6000.00	67.319	7.894	75.213	6.404	47365.2	67.665

This table was computed for the ground electronic state ($^2\Sigma$) using a molecular weight of 88.62797 and the following molecular constants (in cm^{-1}): $\omega_e = 1206.2$, $x_e\omega_e = 17$, $B_e = 3.6751$, $\alpha_e = 0.0814$, $\beta_e = 5.5(10^{-6})$, $D_e = 1.349(10^{-4})$, D_0 (dissociation energy) = 13,500.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-99. Thermodynamic Functions for BaH(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	44.700	6.966	51.667	7.122	1902.8	52.322
298.15	45.311	6.982	52.293	7.193	2081.8	52.293
50.00	32.944	6.890	39.833	6.953	344.5	74.579
75.00	35.742	6.910	42.652	6.951	518.3	63.499
100.00	37.731	6.920	44.652	6.950	692.0	58.549
125.00	39.276	6.926	46.202	6.949	865.8	55.930
150.00	40.539	6.930	47.470	6.951	1039.5	54.418
175.00	41.608	6.934	48.542	6.961	1213.4	53.504
200.00	42.534	6.938	49.472	6.982	1387.7	52.943
225.00	43.352	6.945	50.297	7.017	1562.6	52.604
250.00	44.084	6.955	51.038	7.066	1738.6	52.411
275.00	44.747	6.967	51.715	7.127	1916.0	52.317
300.00	45.354	6.984	52.338	7.198	2095.1	52.293
325.00	45.914	7.003	52.917	7.276	2276.0	52.319
350.00	46.434	7.025	53.459	7.357	2458.9	52.382
375.00	46.919	7.050	53.970	7.440	2643.8	52.471
400.00	47.375	7.077	54.452	7.522	2830.9	52.580
425.00	47.805	7.106	54.911	7.603	3019.9	52.703
450.00	48.212	7.136	55.348	7.681	3211.0	52.838
475.00	48.599	7.166	55.765	7.756	3404.0	52.981
500.00	48.967	7.198	56.165	7.827	3598.8	53.131
550.00	49.656	7.261	56.917	7.958	3993.5	53.441
600.00	50.290	7.324	57.614	8.073	4394.3	53.760
650.00	50.879	7.385	58.265	8.175	4800.5	54.082
700.00	51.429	7.445	58.874	8.263	5211.5	54.403
750.00	51.944	7.502	59.447	8.341	5626.7	54.720
800.00	52.430	7.557	59.987	8.410	6045.5	55.032
850.00	52.890	7.609	60.499	8.470	6467.5	55.339
900.00	53.326	7.658	60.984	8.524	6892.4	55.639
950.00	53.742	7.705	61.447	8.572	7319.8	55.933
1000.00	54.138	7.750	61.887	8.615	7749.5	56.220
1050.00	54.517	7.792	62.309	8.654	8181.3	56.500
1100.00	54.880	7.832	62.712	8.689	8614.8	56.773
1150.00	55.229	7.870	63.099	8.721	9050.1	57.040
1200.00	55.565	7.906	63.471	8.750	9486.9	57.300
1250.00	55.889	7.940	63.829	8.778	9925.1	57.554
1300.00	56.201	7.973	64.173	8.803	10364.6	57.802
1350.00	56.502	8.004	64.506	8.826	10805.4	58.044
1400.00	56.794	8.034	64.827	8.848	11247.2	58.281
1450.00	57.076	8.062	65.138	8.868	11690.1	58.512
1500.00	57.350	8.089	65.439	8.887	12134.0	58.738
1550.00	57.616	8.115	65.731	8.905	12578.8	58.959
1600.00	57.874	8.140	66.014	8.921	13024.5	59.175
1650.00	58.125	8.164	66.289	8.936	13470.9	59.386
1700.00	58.369	8.187	66.556	8.950	13918.1	59.593
1750.00	58.606	8.209	66.815	8.962	14365.9	59.796
1800.00	58.838	8.230	67.068	8.973	14814.3	59.994
1850.00	59.064	8.250	67.314	8.982	15263.1	60.189
1900.00	59.284	8.270	67.554	8.990	15712.4	60.379
1950.00	59.499	8.288	67.787	8.996	16162.1	60.566
2000.00	59.709	8.306	68.015	9.000	16612.0	60.750
2050.00	59.914	8.323	68.237	9.003	17062.1	60.930

Table A-99. Thermodynamic Functions for BaH(gas)-Continued

2100.00	60.115	8.339	68.454	9.004	17512.3	61.106
2150.00	60.311	8.355	68.666	9.003	17962.5	61.280
2200.00	60.504	8.369	68.873	9.000	18412.6	61.450
2250.00	60.692	8.383	69.075	8.995	18862.5	61.617
2300.00	60.876	8.397	69.273	8.989	19312.1	61.781
2350.00	61.057	8.409	69.466	8.980	19761.3	61.943
2400.00	61.234	8.421	69.655	8.969	20210.1	62.102
2450.00	61.408	8.432	69.840	8.957	20658.2	62.258
2500.00	61.578	8.442	70.021	8.942	21105.7	62.411
2600.00	61.910	8.461	70.371	8.907	21998.2	62.711
2700.00	62.229	8.477	70.706	8.865	22886.9	63.001
2800.00	62.538	8.490	71.028	8.817	23771.1	63.281
2900.00	62.836	8.500	71.336	8.762	24650.0	63.554
3000.00	63.124	8.508	71.632	8.702	25523.3	63.818
3100.00	63.403	8.513	71.916	8.636	26390.2	64.075
3200.00	63.674	8.516	72.190	8.567	27250.4	64.324
3300.00	63.936	8.516	72.452	8.494	28103.5	64.567
3400.00	64.190	8.514	72.705	8.419	28949.2	64.802
3500.00	64.437	8.511	72.947	8.341	29787.2	65.032
3600.00	64.677	8.505	73.181	8.262	30617.4	65.255
3700.00	64.909	8.497	73.407	8.182	31439.6	65.472
3800.00	65.136	8.488	73.624	8.101	32253.7	65.684
3900.00	65.356	8.477	73.833	8.020	33059.7	65.890
4000.00	65.571	8.464	74.035	7.939	33857.7	66.091
4100.00	65.780	8.451	74.230	7.858	34647.5	66.287
4200.00	65.983	8.436	74.419	7.779	35429.4	66.479
4300.00	66.181	8.419	74.601	7.701	36203.4	66.665
4400.00	66.375	8.402	74.777	7.624	36969.6	66.848
4500.00	66.563	8.384	74.947	7.548	37728.1	67.026
4600.00	66.747	8.365	75.112	7.474	38479.2	67.200
4700.00	66.927	8.345	75.272	7.402	39222.9	67.370
4800.00	67.103	8.325	75.427	7.331	39959.5	67.536
4900.00	67.274	8.304	75.578	7.262	40689.2	67.699
5000.00	67.442	8.282	75.724	7.195	41412.0	67.858
5100.00	67.605	8.260	75.866	7.130	42128.3	68.014
5200.00	67.766	8.238	76.004	7.067	42838.2	68.166
5300.00	67.922	8.215	76.138	7.006	43541.8	68.315
5400.00	68.076	8.192	76.268	6.947	44239.5	68.461
5500.00	68.226	8.169	76.395	6.890	44931.3	68.604
5600.00	68.373	8.146	76.519	6.834	45617.5	68.744
5700.00	68.517	8.122	76.639	6.780	46298.2	68.882
5800.00	68.658	8.099	76.757	6.729	46973.6	69.017
5900.00	68.796	8.075	76.871	6.678	47643.9	69.149
6000.00	68.931	8.052	76.983	6.630	48309.3	69.278

This table was computed for the ground electronic state ($^2\Sigma$) using a molecular weight of 138.34797 and the following molecular constants (in cm^{-1}): $\omega_e = 1172$, $x_e\omega_e = 16$, $B_e = 3.3823$, $\alpha_e = 0.0655$, $D_e = 1.12(10^{-4})$, D_0 (dissociation energy) = 14,680.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

Table A-100. Thermodynamic Functions for LiO(gas)

T K	-(F-H0)/T	(H-H0)/T	S	CP	(H-H0)	-(F-H298)/T
273.15	42.592	7.108	49.699	7.584	1941.4	50.399
298.15	43.216	7.153	50.369	7.701	2132.5	50.369
50.00	30.763	6.930	37.693	6.955	346.5	73.414
75.00	33.575	6.938	40.513	6.955	520.4	62.008
100.00	35.571	6.943	42.514	6.960	694.3	56.897
125.00	37.121	6.948	44.069	6.983	868.5	54.181
150.00	38.389	6.958	45.346	7.035	1043.7	52.605
175.00	39.462	6.975	46.437	7.119	1220.5	51.648
200.00	40.395	6.999	47.394	7.226	1399.8	51.058
225.00	41.221	7.031	48.252	7.347	1582.0	50.699
250.00	41.964	7.069	49.033	7.471	1767.2	50.494
275.00	42.640	7.111	49.751	7.593	1955.5	50.394
300.00	43.260	7.156	50.416	7.709	2146.8	50.369
325.00	43.835	7.203	51.038	7.816	2340.9	50.397
350.00	44.370	7.250	51.620	7.914	2537.5	50.463
375.00	44.872	7.297	52.170	8.003	2736.5	50.559
400.00	45.345	7.344	52.689	8.083	2937.6	50.676
425.00	45.791	7.390	53.181	8.155	3140.6	50.809
450.00	46.215	7.434	53.649	8.219	3345.3	50.954
475.00	46.618	7.477	54.095	8.277	3551.5	51.108
500.00	47.003	7.518	54.521	8.329	3759.1	51.268
550.00	47.723	7.596	55.319	8.417	4177.8	51.600
600.00	48.387	7.667	56.054	8.488	4600.5	51.941
650.00	49.003	7.733	56.736	8.547	5026.4	52.284
700.00	49.579	7.793	57.371	8.596	5455.0	52.625
750.00	50.118	7.848	57.966	8.636	5885.9	52.961
800.00	50.626	7.898	58.524	8.670	6318.5	53.292
850.00	51.106	7.944	59.051	8.699	6752.8	53.615
900.00	51.562	7.987	59.549	8.723	7188.3	53.931
950.00	51.995	8.026	60.021	8.744	7625.0	54.239
1000.00	52.407	8.063	60.470	8.762	8062.7	54.540
1050.00	52.802	8.096	60.898	8.778	8501.2	54.833
1100.00	53.179	8.128	61.307	8.792	8940.5	55.118
1150.00	53.541	8.157	61.698	8.804	9380.4	55.395
1200.00	53.889	8.184	62.073	8.815	9820.9	55.666
1250.00	54.223	8.210	62.433	8.825	10261.9	55.929
1300.00	54.546	8.233	62.779	8.833	10703.4	56.186
1350.00	54.857	8.256	63.113	8.841	11145.2	56.436
1400.00	55.157	8.277	63.434	8.848	11587.5	56.681
1450.00	55.448	8.297	63.745	8.854	12030.0	56.919
1500.00	55.730	8.315	64.045	8.860	12472.9	57.151
1550.00	56.003	8.333	64.336	8.865	12916.0	57.379
1600.00	56.268	8.350	64.617	8.870	13359.4	57.600
1650.00	56.525	8.365	64.890	8.874	13803.0	57.817
1700.00	56.775	8.380	65.155	8.878	14246.7	58.029
1750.00	57.018	8.395	65.413	8.881	14690.7	58.236
1800.00	57.255	8.408	65.663	8.885	15134.9	58.439
1850.00	57.485	8.421	65.906	8.888	15579.2	58.638
1900.00	57.710	8.433	66.143	8.890	16023.6	58.832
1950.00	57.929	8.445	66.374	8.893	16468.2	59.023
2000.00	58.143	8.456	66.599	8.895	16912.9	59.209
2050.00	58.352	8.467	66.819	8.898	17357.7	59.392

Table A-100. Thermodynamic Functions for LiO(gas)-Continued

2100.00	58.556	8.477	67.034	8.900	17802.7	59.572
2150.00	58.756	8.487	67.243	8.902	18247.7	59.748
2200.00	58.951	8.497	67.448	8.903	18692.8	59.920
2250.00	59.142	8.506	67.648	8.905	19138.0	60.090
2300.00	59.329	8.514	67.844	8.906	19583.3	60.256
2350.00	59.512	8.523	68.035	8.908	20028.7	60.420
2400.00	59.692	8.531	68.223	8.909	20474.1	60.580
2450.00	59.868	8.539	68.406	8.910	20919.6	60.738
2500.00	60.040	8.546	68.586	8.911	21365.1	60.893
2600.00	60.376	8.560	68.936	8.913	22256.4	61.196
2700.00	60.699	8.573	69.272	8.915	23147.8	61.489
2800.00	61.011	8.585	69.597	8.915	24039.3	61.773
2900.00	61.313	8.597	69.909	8.916	24930.8	62.048
3000.00	61.604	8.607	70.212	8.916	25822.4	62.315
3100.00	61.887	8.617	70.504	8.915	26713.9	62.575
3200.00	62.160	8.627	70.787	8.913	27605.3	62.827
3300.00	62.426	8.635	71.061	8.910	28496.5	63.072
3400.00	62.684	8.643	71.327	8.907	29387.3	63.311
3500.00	62.934	8.651	71.585	8.902	30277.7	63.544
3600.00	63.178	8.658	71.836	8.896	31167.7	63.771
3700.00	63.416	8.664	72.080	8.889	32056.9	63.992
3800.00	63.647	8.670	72.317	8.881	32945.4	64.208
3900.00	63.872	8.675	72.547	8.871	33833.0	64.419
4000.00	64.092	8.680	72.772	8.860	34719.6	64.625
4100.00	64.306	8.684	72.990	8.847	35605.0	64.826
4200.00	64.515	8.688	73.203	8.833	36489.0	65.023
4300.00	64.720	8.691	73.411	8.817	37371.5	65.216
4400.00	64.920	8.694	73.613	8.800	38252.3	65.404
4500.00	65.115	8.696	73.811	8.781	39131.4	65.589
4600.00	65.306	8.697	74.004	8.760	40008.4	65.770
4700.00	65.493	8.699	74.192	8.738	40883.4	65.947
4800.00	65.676	8.699	74.376	8.715	41756.0	66.121
4900.00	65.856	8.699	74.555	8.689	42626.2	66.291
5000.00	66.032	8.699	74.730	8.663	43493.9	66.458
5100.00	66.204	8.698	74.902	8.635	44358.8	66.622
5200.00	66.373	8.696	75.069	8.606	45220.8	66.783
5300.00	66.538	8.694	75.233	8.575	46079.9	66.941
5400.00	66.701	8.692	75.393	8.544	46935.9	67.096
5500.00	66.860	8.689	75.549	8.511	47788.7	67.248
5600.00	67.017	8.685	75.702	8.477	48638.1	67.398
5700.00	67.170	8.681	75.852	8.443	49484.1	67.545
5800.00	67.321	8.677	75.998	8.407	50326.6	67.689
5900.00	67.470	8.672	76.142	8.371	51165.5	67.831
6000.00	67.615	8.667	76.282	8.334	52000.8	67.971

This table was computed for the ground electronic state (assumed to be $^2\pi$ but with no doublet separation) for the harmonic oscillator-rigid rotator approximation using a molecular weight of 22.93840 and the following molecular constants (in cm^{-1}): $\omega_e = 745$, $B_e = 1.3300$, D_0 (dissociation energy) = 28,000.

The table is in units of calories, moles, and °K, and for the ideal gas at a standard state of 1 atm. pressure.

APPENDIX II

FUNDAMENTAL CONSTANTS FOR PHYSICAL CHEMISTRY

(Based upon values accepted by the International Union of Pure and Applied Physics and the International Union of Pure and Applied Chemistry, and recommended by the National Academy of Sciences-National Research Council. See the report by J. W. M. DuMond and E. R. Cohen, presented at the Second International Conference on Nuclidic Masses and Atomic Constants in Vienna in July, 1963.)

A. "Defined" Constants

Absolute temperature of the triple point of water	T(triple point)	273.16°K
Standard acceleration of gravity	g_n	980.665 cm sec^{-2}
Standard atmosphere	atm	1,013,250 dynes cm^{-2}
Thermochemical calorie	cal	4.184 joules
International Steam calorie	ITcal	4.1868 joules
British Thermal Unit	BTU/lb	(1/1.8) ITcal g^{-1}
Inch	in	2.54 cm
Pound(avoirdupois)	lb	453.59237 g
Atomic mass unit	u	Exactly 1/12 the mass of an atom of carbon - 12 (^{12}C)
Mole	mol	The amount of substance containing a number of units, atoms or molecules as appropriate for the substance, equal to the number of atoms of carbon - 12 (^{12}C) in exactly 12 grams of pure carbon - 12 (^{12}C).

B. "Basic" Constants

Velocity of light	c	$(2.997925 \pm 0.00003) \times 10^{10}$ cm sec^{-1}
Avogadro number	N	$(6.02252 \pm 0.00028) \times 10^{23}$ molecules mole^{-1}
Faraday constant	$\mathcal{F}$	96487.0 ± 1.6 coulombs equivalent^{-1}
Planck constant	h	$(6.6256 \pm 0.0005) \times 10^{-27}$ erg sec

APPENDIX II (continued)

Pressure-volume product of one mole of gas at zero pressure and 273.15°K(0°C)	$(PV)^{P=0}_{0°C}$	$22413.6 \pm 1.2^{*}$ cm^3 atm mole^{-1} $2271.06 \pm 0.12^{*}$ joules mole^{-1} $542.796 \pm 0.029^{*}$ cal mole^{-1}

C. "Derived" constants

Gas constant per mole	$R = \dfrac{(PV)^{P=0}_{0°C}}{T_{0°C}}$	$8.31433 \pm 0.00044^{*}$ joules deg^{-1} mole^{-1} $1.98717 \pm 0.00011^{*}$ cal deg^{-1} mole^{-1} $82.0561 \pm 0.0043^{*}$ cm^3 atm deg^{-1} mole^{-1}
Boltzmann constant	$k = R/N$	$(1.38054 \pm 0.00011)^{*}$ x 10^{-16} erg deg^{-1} molecule^{-1}
Second radiation constant	$c_2 = hc/k$	1.43879 ± 0.00015 cm deg
Constant relating mass and energy	$Y = c^2$	(8.987554 ± 0.000018) x 10^{13} joules g^{-1}
Constant relating wave number and energy	$Z = Nhc$	11.9626 ± 0.0011 joule cm mole^{-1} 2.85912 ± 0.00026 cal cm mole^{-1}
Constant relating electron-volts per molecule (eV) and energy	$\mathcal{F}/Z$	8065.73 ± 0.23 cm^{-1} (eV)$^{-1}$ 23060.9 ± 0.4 cal mole^{-1} (eV)$^{-1}$

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*The uncertainties assigned to these quantities are somewhat less than those given in the original report.

APPENDIX III

SELECTED THERMOCHEMICAL VALUES

William H. Evans

The following tables represent a preliminary selection from the data prepared for the forthcoming revision of NBS Circular 500, Selected Values of Chemical Thermodynamic Properties. As this work is still in progress, these values are subject to change. It should especially be noted that these tables are not consistent with the earlier tables in Circular 500; care should be used if data from several sources are to be combined.

These preliminary tables are presented here both to make available newer data for compounds of interest and in the hope that errors may be detected and thus corrected before the final version appears.

"Selected Thermochemical Values"

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
O	g	58.983	59.555	55.388	38.467	5.237
O^+	g	373.010	375.070			
O^-	g	25.20	26.68			
O_2	g	0	0	0	48.996	7.016
std state, m = 1	aq		-2.8	3.9	26.5	
O_2^+	g	280.0	281.48			
O_3	g	34.74	34.1	39.0	57.08	9.37
H	g	51.626	52.095	48.580	27.391	4.9679
D	g	52.524	52.981	49.360	29.455	4.9679
H^+	g	365.211	367.161			
std state, m = 1	aq		0	0	0	0
H^-	g	34.40	33.38			
H_2	g	0	0	0	31.208	6.889
D_2	g	0	0	0	34.620	6.978
HD	g	0.079	0.076	-0.350	34.343	6.978
H_2	aq		-1.0	4.2	13.8	
H_2^+	g	355.74	357.22			
OH	g	9.25	9.31	8.18	43.890	7.143
OD	g	8.72	8.81	7.76	45.321	7.140
OH^-	g	-55.7	-57.2			
OH^- std state, m = 1	aq		-54.970	-37.594	-2.57	-35.5
HO_2	g	6.	5.			
HO_2^+	g	272.	271.			
HO_2^- std state, m = 1	aq		-38.32	-16.1	5.7	
H_2O	l		-68.315	-56.688	16.71	17.995
D_2O	l		-70.411	-58.196	18.15	20.16
HDO	l		-69.285	-57.818	18.95	
H_2O	g	-57.102	-57.796	-54.635	45.104	8.025
D_2O	g	-58.855	-59.560	-56.060	47.378	8.19
HDO	g	-57.927	-58.628	-55.720	47.658	8.08
H_2O^+	g	233.5	234.2			
H_2O_2	l		-44.88	-28.78	26.2	21.3
	g	-31.07	-32.58	-25.25	55.6	10.3
std state, m = 1	aq		-45.69	-32.05	34.4	

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
0.5 H_2O	aq		-45.198			
1 H_2O	aq		-45.365			
5 H_2O	aq		-45.638			
10 H_2O	aq		-45.670			
50 H_2O	aq		-45.687			
$H_2O_2^+$	g	220.7	220.7			
F	g	18.38	18.88	14.72	37.917	5.436
F^+	g	420.16	422.14			
F^-	g	-63.6	-65.1			
std state, m = 1	aq		-79.50	-66.64	-3.3	-25.5
F_2	g	0	0	0	48.44	7.48
F_2^+	g	365.1	366.6			
FO	g	54.	54.			
F_2O	g	-5.7	-5.2	-1.1	59.11	10.35
F_2O_2	g		4.3			
F_2O_3	g		38			
HF	l		-71.65		18.02+X	12.35
	g	-64.788	-64.8	-65.3	41.50	6.95
std state, m = 1 undissociated	aq		-76.50	-70.95	21.2	
std state, m = 1 dissociated	aq		-79.50	-66.64	-3.3	-25.5
2 H_2O	aq		-75.79			
3 H_2O	aq		-75.98			
5 H_2O	aq		-76.165			
10 H_2O	aq		-76.235			
25 H_2O	aq		-76.292			
50 H_2O	aq		-76.316			
100 H_2O	aq		-76.340			
200 H_2O	aq		-76.358			
300 H_2O	aq		-76.374			
500 H_2O	aq		-76.423			
700 H_2O	aq		-76.463			
1000 H_2O	aq		-76.531			
2000 H_2O	aq		-76.80			
3000 H_2O	aq		-76.95			
5000 H_2O	aq		-77.14			
10000 H_2O	aq		-77.25			

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
HF_2^- std state, m = 1	aq		-155.34	-138.18	22.1	
XeF_4	c		-62.5			
Cl	g	28.68	29.082	25.262	39.457	5.22
Cl^+	g	328.86	330.74			
Cl^-	g	-57.9	-58.9			
std state, m = 1	aq		-39.952	-31.372	13.5	-32.6
Cl_2	g	0	0	0	53.29	8.10
std state, m = 1	aq		-5.6	1.65	29.	
CCl_4, std state, $N_2 = 1$			-4.44	1.09	34.7	
Cl_2^+	g	264.8	266.3			
ClO	g	24.36	24.34	23.46	54.14	7.52
ClO^- std state, m = 1	aq		-25.6	-8.8	10.	
ClO_2	g	25.09	24.5	28.8	61.36	10.03
std state, m = 1	aq		17.9	28.1	41.4	
ClO_2^- std state, m = 1	aq		-15.9	4.1	24.2	
ClO_3	g		37.			
ClO_3^- std state, m = 1	aq		-23.7	-0.8	38.8	
ClO_4^- std state, m = 1	aq		-30.9	-2.06	43.5	
Cl_2O	g	19.71	19.2	23.4	63.60	10.85
CCl_4, std state, $N_2 = 1$			12.62	22.98	43.0	
Cl_2O_7	g		65.0			
	l		56.9			
HCl	g	-22.016	-22.062	-22.744	44.64	6.95
std state, m = 1	aq		-39.952	-31.372	13.5	-32.6
2 H_2O	aq		-33.69			
3 H_2O	aq		-35.49			
4 H_2O	aq		-36.548			
5 H_2O	aq		-37.231			
8 H_2O	aq		-38.242			
10 H_2O	aq		-38.556			
15 H_2O	aq		-38.964			
25 H_2O	aq		-39.278			
50 H_2O	aq		-39.521			
100 H_2O	aq		-39.657			
500 H_2O	aq		-39.812			
1000 H_2O	aq		-39.850			

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
HCl 5000 H_2O	aq		-39.905			
10000 H_2O	aq		-39.918			
50000 H_2O	aq		-39.936			
CCl_4, std state, $N_2 = 1$			-24.7	-20.3	25.2	
$CHCl_3$, std state, $N_2 = 1$			-25.1	-20.5	24.6	
HClO std state, m = 1 undissociated	aq		-28.9	-19.1	35.	
10 H_2O	aq		-28.62			
100 H_2O	aq		-28.90			
200 H_2O	aq		-28.92			
1000 H_2O	aq		-28.93			
$HClO_2$ std state, m = 1 undissociated			-12.4	6.8	45.0	
$HClO_3$ std state, m = 1	aq		-23.7	-0.8	38.8	
$HClO_4$	l		-9.70			
std state, m = 1	aq		-30.91	-2.06	43.5	
$HClO_4 \cdot H_2O$	c		-91.35			
$HClO_4 \cdot 2H_2O$	l		-162.04			
ClF	g	-11.9	-11.92	-12.28	52.06	7.66
ClF_3	g	-37.0	-38.0	-28.4	67.28	15.26
	l		-44.3			
$(ClF_3)_2$	g		-79.9	-54.7	114.	
ClO_3F	g	-3.6	-5.7	11.5	66.65	15.52
$ClF_3 \cdot HF$	g		-107.5	-90.8	83.	
Br	g		26.740	23.018	41.805	4.968
Br^+	g		301.41			
Br^-	g		-55.9			
std state, m = 1	aq		-29.05	-24.85	19.7	-33.9
Br_2(l)	l		0	0	36.384	18.090
	g		7.387	0.749	58.65	8.62
std state, m = 1	aq		-0.62	0.94	31.2	
CCl_4, std state, $N_2 = 1$			0.71	0.36	37.6	
Br_2^+	g		253.5			
Br_3^- std state, m = 1	aq		-31.17	-25.59	51.5	
Br_5^- std state, m = 1	aq		-34.0	-24.8	75.7	

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
BrO^- std state, m = 1	aq		-22.5	-8.0	10.	
BrO_2	g		-13.4			
BrO_3^- std state, m = 1	aq		-20.0	+0.4	39.0	
HBr	g		-8.70	-12.77	47.437	6.964
std state, m = 1	aq		-29.05	-24.84	19.7	-33.9
1 H_2O	aq		-17.38			
2 H_2O	aq		-22.40			
3 H_2O	aq		-24.68			
4 H_2O	aq		-25.961			
5 H_2O	aq		-26.706			
8 H_2O	aq		-27.649			
10 H_2O	aq		-27.953			
15 H_2O	aq		-28.307			
25 H_2O	aq		-28.540			
50 H_2O	aq		-28.719			
100 H_2O	aq		-28.815			
500 H_2O	aq		-28.926			
1000 H_2O	aq		-28.958			
5000 H_2O	aq		-29.006			
10000 H_2O	aq		-29.019			
50000 H_2O	aq		-29.037			
CCl_4, std state, $N_2 = 1$			-11.9	-10.9	30.4	
$CHCl_3$, std state, $N_2 = 1$			-12.0	-11.0	30.4	
HBrO std state, m = 1 undissociated	aq		-27.0	-19.7	34.	
$HBrO_3$ std state, m = 1	aq		-20.0	+0.4	39.0	
400 H_2O	aq		-19.94			
BrF_3	l		-71.9	-57.5	42.6	29.78
	g		-61.09	-54.83	69.89	15.92
BrF_5	l		-109.6	-84.1	53.8	
	g		-102.5	-83.8	76.50	23.81
BrCl	g		3.50			
CCl_4			-1.547			
I	g	25.631	25.535	16.798	43.184	4.968
I^+	g	266.77	268.16			

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
I^-	g	-45.4	-47.0			
std state, m = 1	aq		-13.19	-12.33	26.6	-34.0
I_2	c	0	0	0	27.757	13.010
	g	15.659	14.923	4.627	62.28	
std state, m = 1	aq		5.4	3.92	32.8	
CCl_4, std state, $N_2 = 1$			6.0	2.66	39.0	
C_6H_6, std state, $N_2 = 1$			4.3	1.7	36.5	
I_3^- std state, m = 1	aq		-12.3	-12.3	57.2	
IO^- std state, m = 1	aq		-25.7	-9.2	-1.3	
IO_3^- std state, m = 1	aq		-52.9	-30.6	28.3	
IO_4^+	aq		-35.2			
I_2O_5	c		-37.78			
HI	g		6.33	0.51	49.351	6.969
std state, m = 1	aq		-13.19	-12.33	26.6	-34.0
3 H_2O	aq		-8.56			
4 H_2O	aq		-10.23			
5 H_2O	aq		-11.09			
6 H_2O	aq		-11.56			
8 H_2O	aq		-12.075			
10 H_2O	aq		-12.335			
25 H_2O	aq		-12.854			
50 H_2O	aq		-12.956			
100 H_2O	aq		-13.014			
500 H_2O	aq		-13.082			
1000 H_2O	aq		-13.106			
5000 H_2O	aq		-13.149			
10000 H_2O	aq		-13.161			
50000 H_2O	aq		-13.178			
HIO std state, m = 1, undissociated	aq		-33.0	-23.7	22.8	
HIO_3	c		-55.0			
std state, m = 1 undissociated	aq		-50.5	-31.7	39.9	
100 H_2O	aq		-51.7			
800 H_2O	aq		-52.2			

Substance	State	ΔHf°$_0$	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
IF_5	l		-206.7			
	g	-194.29	-196.58	-179.68	78.3	23.7
IF_7	g	-227.4	-225.6	-195.6	82.8	32.6
ICl α	c		-8.4			
	l		-5.71	-3.25	32.3	
	g		4.25	-1.30	59.15	
std state, m = 1	aq			-4.1		
CCl_4, std state $N_2 = 1$			-3.3	-2.1	36.5	
ICl_3	c		-21.	-5.34	40.0	
IBr	c		-2.5			
	g		9.76	0.89	61.84	
std state, m = 1	aq			-1.0		
CCl_4, std state, $N_2 = 1$			1.62	-0.4	39.	
S rhombic	c	0	0	0	7.60	5.41
monoclinic			0.08			
	g	66.1	66.636	56.949	40.094	5.658
$6CS_2$			0.405			
S^+	g	304.95	306.97			
S^-	g	18.36	-17.42			
S^{--} std state, m = 1	aq		7.9	20.5	-3.5	
S_2	g	30.65	30.68			
S_3	g		31.7			
S_4	g		32.7			
S_5	g		29.6			
S_6	g		24.5			
S_7	g		27.1			
S_8	g	25.35	24.45	11.87	102.98	37.39
SO	g	1.5				
SO_2	l		-76.6			
	g	-70.336	-70.944	-71.749	59.30	9.53
std state, m = 1 undissociated	aq		-77.194	-71.872	38.7	
100 H_2O	aq		-78.054			
200 H_2O	aq		-78.355			
500 H_2O	aq		-78.811			

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
SO_2 1000 H_2O	aq		-79.201			
2000 H_2O	aq		-79.642			
5000 H_2O	aq		-80.209			
10000 H_2O	aq		-80.584			
SO_3 β	c		-108.63	-88.19	12.5	
	l		-105.41	-88.04	22.85	
	g	-93.21	-94.58	-88.69	61.34	12.11
SO_3^{--} std state, m = 1	aq		-151.9	-116.3	-7.	
SO_4^{--} std state, m = 1	aq		-217.32	-177.97	4.8	-70.
$S_2O_3^{--}$	aq		-155.9			
$S_2O_8^{--}$ std state, m = 1	aq		-320.0	-265.4	59.3	
HS^- std state, m = 1	aq		-4.2	-2.88	15.0	
H_2S	g	-4.381	-4.93	-8.02	49.16	8.18
std state, m = 1 undissociated	aq		-9.5	-6.66	29.	
HSO_3^- std state, m = 1 undissociated	aq		-149.67	-126.15	33.4	
HSO_4^- std state, m = 1 undissociated	aq		-212.08	-180.69	31.5	-20.
H_2SO_3 std state, m = 1 undissociated	aq		-145.51	-128.56	55.5	
H_2SO_3 100 H_2O	aq		-146.369			
200 H_2O	aq		-146.670			
500 H_2O	aq		-147.126			
1000 H_2O	aq		-147.516			
2000 H_2O	aq		-147.957			
5000 H_2O	aq		-148.524			
10000 H_2O	aq		-148.899			
H_2SO_4	c	-194.019				
	l		-194.548	-164.942	37.501	33.20
std state, m = 1	aq		-217.32	-177.97	4.8	-70.
1 H_2O	aq		-201.193			
2 H_2O	aq		-204.425			
3 H_2O	aq		-206.241			
4 H_2O	aq		-207.428			
5 H_2O	aq		-208.288			

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
H_2SO_4 6 H_2O	aq		-208.944			
8 H_2O	aq		-209.865			
10 H_2O	aq		-210.451			
15 H_2O	aq		-211.191			
25 H_2O	aq		-211.660			
50 H_2O	aq		-211.941			
75 H_2O	aq		-212.068			
100 H_2O	aq		-212.150			
115 H_2O	aq		-212.192			
200 H_2O	aq		-212.387			
300 H_2O	aq		-212.565			
500 H_2O	aq		-212.833			
800 H_2O	aq		-213.128			
1000 H_2O	aq		-213.275			
1500 H_2O	aq		-213.552			
2000 H_2O	aq		-213.740			
3000 H_2O	aq		-214.015			
5000 H_2O	aq		-214.390			
10000 H_2O	aq		-215.060			
20000 H_2O	aq		-215.880			
50000 H_2O	aq		-216.545			
100000 H_2O	aq		-216.875			
500000 H_2O	aq		-217.189			
$H_2SO_4 \cdot H_2O$	1		-269.508	-227.186	50.56	51.35
$H_2S_2O_7$	c		-304.4			27.
$H_2S_2O_8$ std state, m=1	aq		-320.0	-265.4	59.3	
SF_4	g	-183.4	-185.2	-174.8	69.77	17.45
SF_6	g	-285.7	-289.	-264.1	69.72	23.25
SOF_2	g				59.71	13.58
SO_2F_2	g				61.00	15.78
S_2Cl_2	1		-14.2			
	g	-4.18	-4.4	-7.6	79.2	17.6
$SOCl_2$	1		-58.7			29.
	g	-50.07	-50.8	-47.4	74.0	15.9

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
SO_2Cl_2	l		-94.2			32.
	g		-87.0			
$S_2O_5Cl_2$	l		-168.7			56.
	g		-153.2			
SF_5Cl	g	-247.48	-250.5	-226.9	76.26	24.9
Se hexagonal, black	c	0	0	0	10.144	6.062
monoclinic, red	c		1.6			
amorphous, glassy	am		1.2			
Se_2	g		34.9			
Se_6	g		48.7			
SeO_2	c		-53.86			
	aq		-57.97			
SeO_3	c		-39.9			
SeO_3^{--} std state, m = 1	aq		-121.7	-88.4	3.	
SeO_4^{--} std state, m=1	aq		-143.2	-105.5	12.9	
HSe^- std state, m = 1 undissociated	aq		3.8	10.5	19.	
H_2Se	g	8.05	7.1	3.8	52.32	8.30
std state, m = 1 undissociated	aq		4.6	5.3	39.1	
$HSeO_3^-$ std state, m = 1 undissociated	aq		-127.98	-98.36	33.1	
$HSeO_4^-$ std state, m = 1 undissociated	aq		-139.0	-108.1	35.7	
H_2SeO_3	c		-125.35			
std state, m = 1 undissociated	aq		-121.29	-101.87	49.7	
	aq		-121.34			
H_2SeO_4	c		-126.7			
1200 H_2O	aq		-140.3			
$H_2SeO_4 \cdot H_2O$	c		-200.9			
	l		-196.1			
SeF_6	g	-243.1	-246.	-222.	74.99	26.4
Se_2Cl_2	l		-19.7			
	g		4.			
Te	c	0	0	0	11.88	6.15
	amorph		2.7			

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
Te_2	g	40.7	40.2			
TeO_2	c		-77.	-64.6	19.0	
TeO_3^{--}	aq		-142.6			
H_2Te	g		23.8			
H_2TeO_3	aq		-76.2			
$Te(OH)_3^+$ std state, m=1	aq		-145.4	-118.6	26.7	
$H_4TeO_6^{--}$	aq		-292.1			
$H_5TeO_6^-$	aq		-301.5			
H_6TeO_6	c		-310.4			
	aq		-307.			
TeF_6	g		-315.			
$TeCl_4$	c		-78.0			33.1
$TeBr_4$	c		-45.5			
N	g	112.534	112.979	108.883	36.622	4.968
N^+	g	447.663	449.589			
N_2	g	0	0	0	45.77	6.961
N_3^+	g	389.	390.2			
N_3^-	g	45.	43.2			
std state, m = 1	aq		65.76	83.2	25.8	
NO	g	21.45	21.57	20.69	50.35	
NO^+	g	234.8	236.4			
NO_2	g	8.60	7.93	12.26	57.35	8.89
NO_2^+	g	276.6	277.4			
NO_2^- std state, m = 1	aq		-25.0	-8.9	33.5	-23.3
NO_3^- std state, m = 1	aq		-49.56	-26.61	35.0	-20.7
N_2O	g	20.435	19.61	24.90	52.52	9.19
N_2O_3	1		12.02			
	g	21.628	20.01	33.32	74.61	15.68
N_2O_4	1		-4.66	23.29	50.0	34.1
	g	4.49	2.19	23.38	72.70	18.47
N_2O_5	c		-10.3	27.2	42.6	34.2
	g	5.7	2.7	27.5	85.0	20.2
NH	g	79.	80.			
NH_2	g		41.			
NH_3	g	-9.34	-11.07	-3.94	45.97	8.38

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
NH_3 std state, m = 1 undissociated	aq		-19.19	-6.35	26.6	
1 H_2O	aq		-18.011			
2 H_2O	aq		-18.560			
5 H_2O	aq		-18.945			
10 H_2O	aq		-19.074			
20 H_2O	aq		-19.125			
50 H_2O	aq		-19.156			
100 H_2O	aq		-19.167			
500 H_2O	aq		-19.173			
1000 H_2O	aq		-19.171			
5000 H_2O	aq		-19.154			
10000 H_2O	aq		-19.140			
50000 H_2O	aq		-19.086			
NH_4^+ std state, m = 1	aq		-31.67	-18.97	27.1	19.1
N_2H_4	l		12.10	35.67	28.97	23.63
	g	26.18	22.80	38.07	56.97	11.85
std state, m = 1 undissociated	aq		8.20	30.6	33.	
$N_2H_5^+$ std state, m = 1	aq		-1.8	19.7	36.	11.8
HN_3	l		63.1	78.2	33.6	
	g	71.82	70.3	78.4	57.09	10.44
std state, m = 1 undissociated	aq		62.16	76.9	34.9	
HN_3^+	g	309.	308.8			
NH_4N_3	c		27.6	65.5	26.9	
std state, m = 1	aq		34.1	64.3	52.7	
HNO_2(cis)	g	-17.12	-18.64	-10.27	59.43	10.70
(trans)	g	-17.68	-19.15	-10.82	59.54	11.01
(cis-trans mixture)	g		-19.0	-11.0	60.7	10.9
std state, m = 1 undissociated	aq		-28.5	-13.3	36.5	
HNO_3	l		-41.61	-19.31	37.19	26.26
	g	-29.94	-32.28	-17.87	63.64	12.75
std state, m = 1	aq		-49.56	-26.61	35.0	20.7
1 H_2O	aq		-44.845			
2 H_2O	aq		-46.500			
3 H_2O	aq		-47.459			

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
HNO_3 5 H_2O	aq		-48.462			
10 H_2O	aq		-49.192			
25 H_2O	aq		-49.430			
50 H_2O	aq		-49.439			
100 H_2O	aq		-49.440			
500 H_2O	aq		-49.468			
1000 H_2O	aq		-49.484			
5000 H_2O	aq		-49.518			
10000 H_2O	aq		-49.529			
50000 H_2O	aq		-49.545			
NH_2OH	c		-27.3			
	aq		-23.5			
$NH_2OH_2^+$	aq		-32.8			
NH_4OH	l		-86.33	-60.74	39.57	37.02
std state, m = 1 undissociated	aq		-87.505	-63.04	43.3	
std state, m = 1 ionized	aq		-86.64	-56.56	24.5	16.4
NH_4NO_2	c		-61.3			
std state, m = 1	aq		-56.7	-27.9	60.6	-4.2
NH_4NO_3 c,V	c		-87.38	-43.98	36.11	33.3
std state, m = 1	aq		-81.23	-45.58	62.1	-1.6
3 H_2O	aq		-83.485			
5 H_2O	aq		-83.050			
10 H_2O	aq		-82.470			
25 H_2O	aq		-81.866			
50 H_2O	aq		-81.538			
100 H_2O	aq		-81.318			
500 H_2O	aq		-81.183			
1000 H_2O	aq		-81.177			
5000 H_2O	aq		-81.194			
10000 H_2O	aq		-81.202			
$NH_2OH\cdot HNO_3$	c		-87.6			
	aq		-82.4			
N_2H_5OH	l		-58.01			
	g		-49.0	-18.9	63.	

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
N_2H_5OH std state, m=1 undissociated	aq		-60.11	-26.1	49.7	17.5
$N_2H_5NO_3$	c		-60.13			
std state, m = 1	aq		-51.41	-6.91	71.	
NF_2	g	9.68	10.3	13.9	59.71	9.80
NF_3	g	-28.43	-29.8	-20.0	62.29	12.7
N_2F_2 (cis)("active")	g		16.6			
(trans)	g		19.6			
N_2F_4	g	0.88	-1.7	19.4	71.96	18.9
NOF	g	-15.33	-15.9	-12.2	59.27	9.88
NO_2F	g				62.2	11.9
NF_2H	g				60.40	10.37
NH_4F	c	-107.41	-110.89	-83.36	17.20	15.60
std state, m = 1	aq		-111.17	-85.61	23.8	-6.4
$NH_4F \cdot H_2O$	c				-34.92	37.22
NH_4HF_2	c	-187.94	-191.9	-155.6	27.61	25.50
std state, m = 1	aq		-187.01	-157.15	49.2	
4.54 H_2O	aq		-186.8			
NCl_3	l		55.			
NOCl	g	12.82	12.36	15.78	62.52	10.68
NO_2Cl	g	4.29	3.0	13.0	65.02	12.71
$NOClO_4$	c		-36.9			
NO_2ClO_4	c		8.7			
NH_4Cl	c		-75.15	-48.51	22.6	20.1
std state, m = 1	aq		-71.62	-50.34	40.6	-13.5
10 H_2O	aq		-71.567			
50 H_2O	aq		-71.484			
100 H_2O	aq		-71.487			
500 H_2O	aq		-71.528			
1000 H_2O	aq		-71.547			
5000 H_2O	aq		-71.580			
10000 H_2O	aq		-71.591			
N_2H_5Cl	c		-47.0			
std state, m = 1	aq		-41.8	-11.7	49.5	-15.8
$N_2H_5Cl \cdot HCl$	c		-87.8			
$NH_2OH \cdot HCl$	c		-75.9			22.2
	aq		-72.6			

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
NH_4ClO_4	c		-70.58	-21.25	44.5	
std state, m = 1	aq		-62.58	-21.03	70.6	
$N_2H_5ClO_4$	c		-42.2			
std state, m = 1	aq		-32.7	17.6	79.7	
$N_2H_5ClO_4\cdot 1/2H_2O$	c		-78.18			
NOBr	g		19.64	19.70	65.38	10.87
NH_4Br	c		-64.73	-41.9	27.	23.
std state, m = 1	aq		-60.72	-43.69	46.8	-14.8
N_2H_5Br	c		-37.2			
std state, m = 1	aq		-30.8	-5.2	55.7	-17.1
NH_4I	c		-48.14	-26.9	28.	
std state, m = 1	aq		-44.86	-31.30	53.7	-14.9
NH_3NI_3 "nitrogen triiodide"	c		36.9			
NH_4HS	c		-37.5	-12.1	23.3	
200 H_2O	aq		-34.8			
H_2NSO_3H	c		-161.3			
	aq		-156.3			
NH_4HSO_3	c		-183.7			
300 H_2O	aq		-181.3			
NH_4HSO_4	c		-245.45			
200 H2O	aq		-245.65			
$NH_2OH\cdot H_2SO_4$	aq		-246.7			
$(NH_4)_2SO_3$	c		-211.6			
400 H_2O	aq		-211.0			
$(NH_4)_2SO_3\cdot H_2O$	c		-283.8			
$(NH_4)_2SO_4$	c		-282.23	-215.56	52.6	44.81
std state, m = 1	aq		-280.66	-215.77	58.6	-31.8
10 H_2O	aq		-280.72			
50 H_2O	aq		-280.51			
100 H_2O	aq		-280.407			
500 H_2O	aq		-280.242			
1000 H_2O	aq		-280.217			
$(NH_2OH)_2\cdot H_2SO_4$	aq		-281.3			
$(NH_4)_2S_2O_8$	c		-392.5			
	aq		-383.3			

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
$(N_2H_5)_2SO_4$	c		-229.2			
std state, m = 1	aq		-221.0	-138.6	77.	-36
$(N_2H_5)_2SO_4\cdot H_2O$	c		-291.3			
NSF	g				62.07	10.55
NSF_3	g				68.48	17.18
NH_4HSe	c		-31.18	-5.6	23.1	
NH_4Te	c		0.3			
P, α, III, white	c	0	0	0	9.82	5.698
red, triclinic	c	-3.78	-4.2	-2.9	5.45	5.07
black	c		-9.4			
red	amorph		-1.8			
	g				38.978	4.968
in CS_2			0.5			
P_2	g		34.5			
P_4	g	15.83	14.08	5.85	66.89	16.05
PO_3^-	aq		-233.5			
PO_4^{---}, std state, m=1	aq		-305.9	-244.0	-53.	
$P_2O_7^{----}$, std state m = 1	aq		-542.8	-459.8	-25.	
P_4O_6	c		-392.0			
P_4O_{10} hexagonal	c	-705.82	-713.2	-644.8	54.70	50.60
	amorph		-727.			
PH_3	g	3.20	1.3	3.2	50.22	8.87
std state, m = 1	aq		-2.16	0.35	48.2	
PH_3^+	g	243.	242.8			
P_2H_4	l		-1.2			
	g		5.0			
HPO_3	c		-226.7			
	aq		-233.5			
HPO_3^{--}	aq		-229.4			
HPO_4^{--} std state, m = 1	aq		-309.37	-260.91	-8.0	

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
$H_2PO_3^-$	aq		-229.5			
$H_2PO_4^-$ std state, m = 1	aq		-310.88	-270.73	21.6	
H_3PO_2	c		-144.5			
200 H_2O	aq		-144.4			
H_3PO_3	c		-228.3			
	aq		-228.4			
H_3PO_4	c	-301.293	-305.7	-267.5	26.41	25.35
	l		-302.8			
H_3PO_4 std state, m = 1	aq		-307.92	-273.10	37.8	
1 H_2O	aq		-304.69			
1.5 H_2O	aq		-305.26			
2 H_2O	aq		-305.60			
3 H_2O	aq		-306.23			
4 H_2O	aq		-306.60			
5 H_2O	aq		-306.87			
7 H_2O	aq		-307.20			
10 H_2O	aq		-307.48			
20 H_2O	aq		-307.831			
50 H_2O	aq		-308.067			
100 H_2O	aq		-308.176			
200 H_2O	aq		-308.276			
500 H2O	aq		-308.403			
1000 H_2O	aq		-308.532			
2000 H_2O	aq		-308.696			
3000 H_2O	aq		-308.818			
5000 H_2O	aq		-308.982			
10000 H_2O	aq		-309.197			
$H_3PO_4\cdot 1/2\ H_2O$	c	-336.899	-342.1	-296.9	30.87	20.12
$HP_2O_7^{---}$ std state, m=1	aq		-543.7	-472.5	15	
$H_2P_2O_7^{--}$ std state, m=1	aq		-544.6	-481.6	42	

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
$H_3P_2O_7^-$ std state, m =1	aq		-544.1	-484.7	54	
$H_4P_2O_7$	c		-535.6			
supercooled	l		-533.4			
std state, m = 1	aq		-542.2	-486.8	68	
500 H_2O	aq		-543.0			
$H_4P_2O_7 \cdot 3/2H_2O$	c		-640.9			
	l		-637.3			
PF_3	g	-216.05	-217.4	-212.3	65.28	14.03
PF_5	g		-381.4			
POF_3	g	-285.19	-287.3	-275.7	68.11	16.41
PCl_3	l		-74.25	-62.9	51.7	
	g	-65.65	-66.4	-61.8	74.49	17.17
PCl_3^+	g	182.	183.			
PCl_5	c		-106.0			
	g	-86.03	-87.3	-70.7	87.11	26.96
$POCl_3$	c	-145.81				
	l		-142.7	-124.5	53.17	33.17
	g		-133.48	-122.60	77.76	
PH_4Cl	c		-34.7			
$P(OH)_4ClO_4$	c		-325.3			
PBr_3	l		-41.9	-39.8	57.4	
	g		-31.1	-36.7	83.17	18.16
$POBr_3$	c		-109.6			
	g				85.97	21.48
PH_4Br	c		-30.5	-11.4	26.3	
PI_3	c		-10.9			
	g				89.45	18.73
PH_4I	c		-16.7	0.2	29.4	26.2
P_2S_3	c		-19.2			
$PSCl_3$	g				80.47	21.39
$PSBr_3$	c				55.2	
	g				89.07	22.69

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
PN	g				50.437	
$1/n(PN)_n$	c		-15			
P_3N_5	c		-71.4			36.
$NH_4H_2PO_4$	c		-345.94	-289.89	36.32	34.00
std state, m = 1	aq		-342.05	-289.70	48.7	
15 H_2O	aq		-342.157			
50 H_2O	aq		-342.113			
100 H_2O	aq		-342.088			
500 H_2O	aq		-342.059			
1000 H_2O	aq		-342.055			
∞ H_2O	aq		-342.05			
$(NH_4)_2HPO_4$	c		-374.50			45.
std state, m = 1	aq		-372.71	-298.85	46.2	
15 H_2O	aq		-370.40			
50 H_2O	aq		-370.85			
100 H_2O	aq		-371.22			
500 H_2O	aq		-371.4			
1000 H_2O	aq		-371.44			
$(NH_4)_3PO_4$	c		-399.6			
600 H_2O	aq		-391.3			
$(NH_4)_3PO_4 \cdot 3H_2O$	c		-610.8			
C	g	169.98	171.291	160.442	37.760	4.980
diamond	c	0.5797	0.4533	0.6930	-568	1.4615
graphite	c	0	0	0	1.372	2.038
CO	g	-27.200	-26.416	-32.780	42.214	6.965
CO_2	g	-93.964	-94.051	-94.261	51.072	8.874
std state, m = 1 undissociated	aq		-98.85	-92.26	28.3	
CO_3^{--} std state, m = 1	aq		-161.79	-126.17	-13.4	
HCO_3^- std state, m = 1 undissociated	aq		-165.34	-140.26	22.0	
H_2CO_3 std state, m = 1 undissociated	aq		-167.17	-148.94	45.0	

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
		kcal/mole	kcal/mole		cal/deg mole	
Ag	c	0	0	0	10.20	6.10
Ag^+ std state, m = 1	aq		25.234	18.433	17.40	
Ag_2O	c		-7.42	-2.68	29.0	
AgCl	c		-30.370	-26.244	23.0	
$PbCl_2$	c		-85.9	-75.05	32.5	
Na^+ std state, m = 1	aq		-57.39	-62.593	14.1	11.1
NaOH std state, m = 1	aq		-112.36	-100.189	11.5	-24.4
K^+ std state, m = 1	aq		-60.32	-67.70	24.5	5.2
KOH std state, m = 1	aq		-115.29	-105.30	21.9	-30.3
$KClO_3$	c		-93.89		34.17	
std state, m = 1	aq		-84.0	-68.5	63.3	
$KClO_4$	c		-103.43		36.1	26.34
std state, m = 1	aq		-91.23	-69.76	68.0	

APPENDIX IV

PRELIMINARY LIST OF IONIZATION POTENTIALS OR ELECTRON AFFINITIES OF LIGHT ELEMENT COMPOUNDS

Charles W. Beckett

Ionization potentials and electron affinities of a large number of substances are needed for thermodynamic calculations at temperatures from 2000 to 6000°K and higher and involving a fairly large number of elements. Recent reports by Kiser [1] include compilations of the large number of values that are needed. However, these reports do not give selected "best" values that would be most helpful to those who are concerned with thermodynamic calculations.

The table No. 1 below lists ionization potentials and electron affinities for a fairly large group of substances that are likely to occur in at least small amounts in complex mixtures at high temperatures. The first ionization potentials of monatomic gaseous species were obtained in a private communication from Dr. Charlotte M. Sitterly [2]. Many of these values are changed only slightly from values reported in her publications [3]. In most cases slight changes were due to a change in the physical constants used in conversion of reciprocal wave length to electron volts. The new conversion factor is 0.000123981 e.v./cm^{-1}. In a few cases more accurate ionization potentials have become available; however, the changes are small as compared to the errors in the ionization potentials of most other substances.

The ionization potentials and dissociation energies of a number of diatomic molecules have been reviewed critically by P. G. Wilkinson [4]. His values have been adopted for many of the diatomic molecules listed in the table below.

Spectroscopic and photoionization determination of the ionization potentials of a number of polyatomic molecules have been compiled by W. C. Price [5] in a recent issue of the Handbuch der Physik. The ionization potentials of some of the polyatomic molecules given in the table below were taken from this review. In other cases values for polyatomic molecules were obtained by a selection from those listed in the compilation of Kiser [1], with first preference being given to values obtained by photoionization or spectroscopic methods when these data are available. The second preference was electron impact data which are in general less precise and more discordant.

In some cases values for the ionization potentials were obtained from recent literature. The ionization potential of HO_2 and H_2O_2 were reported by S. N. Foner and R. L. Hudson [6]. Verhaegen, Stafford and Drowart [7] have reported ionization potentials for molecules containing boron, carbon, and silicon. Berkowitz and Chupka [8] and Berkowitz and Marquart [9] give ionization potentials for S_8 which differs from earlier values. They give a value for S_6. Nakayama and Watanabe [10] and Dibeler and Reese [11] report very accurate determinations of the ionization potential of acetylene with good agreement with previous measurements. Schoen [12] reports retarding potential measurements of electrons photoemitted by N_2, CO, and O_2 in satisfactory agreement with previous values. J. H. Yang and D. C. Conway [13] report a value for the binding energy of the ion cluster O_4^+ very close to the value obtained for N_4^+ by R. N. Varney [14]. From these data one can compute ionization potentials for the corresponding neutral cluster that may be of some interest in the study of the electrical properties of dense gases. Two recent quantum mechanical studies [15] and [16] yield new values for the binding energy of the H_3^+ ion. When these values are combined with the binding energy of the corresponding neutral molecule [17] and [18], one can obtain the ionization potential of the latter.

The electron affinities of a few monatomic and diatomic species have been determined accurately by Berry and others [19] and [20], and by Branscomb and Smith and their collaborators [21], [22], and [23]. (See also Chantry and Schulz [24]). Edlén [25] and [26] and Clementi and others [27] and [28] give values for electron affinities of monatomic species in the first two rows of the Periodic Table that have been obtained by a combination of quantum mechanical calculation and semi-empirical correlation of isoelectronic series of ions. The recently determined accurate experimental values are listed in the table below where available. Values for the other monatomic negative ions in the first two rows of the Periodic Table were obtained by taking an average of the values by Edlén [25] and [26] and by Clementi and others [27] and [28]. The value given for the electron affinity of monatomic hydrogen has been computed accurately by quantum mechanical methods which have been discussed recently by C. W. Scherr and R. E. Knight [29], [30], and [31], Pekeris [32], and Kinoshita [33]. The total energy in atomic units for the hydrogen negative ion H^- is -0.5277 5101 and the corresponding value for neutral helium He is -2.9037 2434.

D. Cubicciotti [34] has reviewed the earlier electron affinity data from the alkali halides in his Table 7, page 1650. Revised values are given by him in subsequent notes [34].

R. E. Honig [35] has observed negative ions C_1^- to C_8^- in a mass spectrometric study of the sublimation of graphite. He lists relative ion intensities at 2400°K of all of the above species and heats derived from the temperature derivative of the intensities of three species: C_2^-, C_3^-, and C_4^-. From these data he gives the following electron affinities: 1.2 e.v. for C_1, 3.1 to 4.0 e.v. for C_2, 1.8 to 2.5 e.v. for C_3. The value for C_1 is quite close to the recently determined value 1.25 ± .03 e.v. given by M. Seman and L. M. Branscomb [23]. From the relative ion intensities for C_4^- to C_8^- and from data on the neutral molecules from more recent mass spectrometer and theoretical investigations [36], [40], [41], and [42], one may estimate approximate electron affinities for C_4^- to C_8^- which appear to be quite high, about 4 ± 1 e.v. Thus it seems that the polyatomic negative ions of carbon may be significant in many fuel-rich combustion mixtures.

The occurrence of many other negative ions of carbon, hydrogen, and oxygen has been reported in a recent paper on "Negative Ion Mass Spectra of Hydrocarbons and Alcohols," by C. E. Melton and P. S. Rudolph [37]. Relative intensities are given, but electron affinities cannot be obtained from this data, since the experimental conditions do not approach thermodynamic equilibrium. However, the observations suggest that many of these same species could occur in a combustion mixture. Electron affinities of a few additional diatomic and polyatomic molecules or free radicals were taken from the compilation by R. W. Kiser [1].

Time did not permit a comprehensive search of the literature, nor a critical evaluation of the data. It is expected that such work will be carried out during the next few years in connection with a new program, the National Standard Reference Data System. Information concerning this new project on the critical evaluation of ionization potentials of molecules can be obtained by communicating with Dr. H. Rosenstock, Chief, Mass Spectrometry Section, Physical Chemistry Division.

The preparation of this survey was carried out to obtain quickly a preliminary listing of values that would be useful in determining what substances are likely to be important in high-temperature thermodynamic research on mixtures of the lighter elements. Estimates of error are often in themselves of very dubious value and hence should be regarded as provisional.

In addition to the problem of selecting "best" values from discordant literature, there is a high probability that some important substances (i.e., species having ionization potentials less than 6 volts or electron affinities greater than 1/2 volt) may be omitted due to the lack of information. A noteworthy case of this type is discussed in a recent communication by Kistiakowsky and Michael [38] in the Journal of Chemical Physics in which the authors suggest that an unstable hydrocarbon radical C_3H_3 may play an important role in chemi-ionization of hydrocarbom combustion mixtures. They have estimated the ionization potential of the cyclopropene radical, C_3H_3, to be quite low, probably about 3 to 4 e.v. In another communication G. P. Glass and G. B. Kistiakowsky [39] suggest methods of obtaining the corresponding molecule ion $C_3H_3^+$. The stability of the ammonium radical (NH_4) was calculated by D. M. Bishop [43]. He gives 3.94 for the ionization potential of NH_4.

It is a pleasure to acknowledge private communications from Dr. Billings Brown of the Boeing Company, Seattle, Washington, [44] who has conducted a survey entitled, "A Survey of Ionization Potentials of Combustion Products," by L. K. O'Bryan and Billings Brown, July 10, 1964. I should also like to acknowledge information received and helpful discussions with Dr. Charlotte M. Sitterly, Dr. Harold S. Boyne, Dr. William H. Evans, and Dr. Henry Rosenstock, all of whom are interested in the status and needs for ionization potentials and electron affinities.

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Formula	I.P. (or E.A.) e.v.	Est. Error e.v.	
H^-	0.754	0.001	
H	13.598		
H_2	15.426		
H_3	9.0	1.0	
O^-	1.465	0.005	
O	13.618		
O_2^-	0.58	0.1	
O_2	12.075	0.01	
O_4	11.65	0.1	$O_4^+ = O_2 + O_2^+$ + 0.42 e.v.
OH^-	2.7	0.4	
OH	13.36	0.2	
H_2O	12.61	0.02	
HO_2	11.53	0.02	
H_2O_2	10.92	0.05	
F^-	3.448	0.005	
F	17.422		
F_2	15.7	0.2	
HF	15.77	0.2	
OF	13.	0.5	
OF_2	13.7	0.2	

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.
Cl^-	3.613	0.005
Cl	12.97	
Cl_2	11.48	0.05
HCl	12.74	0.01
ClF_3	13.0	0.4
ClO	$\leq$ 10.4	0.2
ClO_3	11.7	
S^-	2.07	0.07
S	10.360	
S_2	8.3	1.
S_8	8.9 (9.6)	1.
SH^-	2.6	0.5
HS	11.1	0.2
H_2S	10.47	0.1
SO	12.1	0.3
SO_2	12.34	0.2
SF_6	16.15	0.5
N^-	0.04	0.04
N	14.53	
N^+	29.59	
N_2	15.580	0.005

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.	
N_3^-	3.13	0.3	
N_4	15.07	0.1	$N_4^+ = N_2 + N_2^+$ 0.5 e.v.
NH	13.10	0.1	
NH_2^-	1.22	0.5	
NH_2	11.6	0.4	
NH_3	10.154	0.05	
NH_4	3.94	1.	(Calculated by D. M. Bishop)
NO	9.267	0.01	
NO^+	30.6	0.3	
NO_2^-			
NO_2	9.78	1.	
N_2O	12.94		
NF	12.2	0.3	
NF_2	11.6	0.5	
NF_3	13.0	0.3	
N_2F_4	12.0	0.3	
NHF_2	12.0	0.3	
P^-	0.77	0.2	
P	10.486		
P_2^-	0.3	0.3	
P_2	11.8	0.5	
P_4	9.0		

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
PH_3	10.1	0.2
PCl_3	12.2	0.2
PH	9.5	0.5
C^-	1.25	0.03
C_2^-	3.1	1.
C_3^-	1.8	1.
C_4^-	4.0	1.
C	11.26	
C_2	12.0	0.4
C_3	12.6	0.4
C_4	12.6	0.4
C_5	12.5	0.4
CH	10.64	0.01
CH_2	10.396	0.01
CH_3	9.84	0.01
CH_4	13.0	0.1
C_2H_2	11.406	0.01
C_2H_4	10.51	0.01
C_2H_6	11.65	0.1
C_6H_6	9.247	0.05
$(C_6H_5)_2$	8.3	0.1
Pyrene	7.55	0.1

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
Coronene	7.6	0.1
CH_3^-	1.1	0.2
$C_6H_6^-$	0.54	0.2
$(C_6H_5)_2^-$	0.41	0.2
$C_{10}H_8^-$	0.65	0.2
CO	14.01	0.01
CO_2	13.79	0.02
CHO	9.85	0.1
CH_2O	10.88	0.04
CH_2O_2	11.33	0.04
CH_4O	10.85	0.04
CF	13.8	0.2
CF_2	13.3	0.2
CF_3	9.7	0.5
CF_4	17.81	0.04
C_2F_4	10.12	0.2
C_6F_6	10.0	0.2
CCl_2F_2	11.7	0.5
CCl	12.9	0.2
CCl_2	13.3	0.2
CCl_3	13.10	0.2
CCl_4	11.47	0.1

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.	
$COCl_2$	11.78	0.04	
CS	11.8	0.3	
CS_2	10.07	0.02	
COS	11.3	0.07	
CN^-	3.21	0.3	
CN	14.2	0.3	
HCN	13.73	0.1	
CNCl	12.49	0.1	
CH_3N_3	9.5	0.2	methyl azide
CH_3ON	10.84	0.1	formamide
CH_3ON	8.2	0.3	methylnitrosyl
CH_3O_2N	11.08	0.04	
CH_5N	8.97	0.04	methyl amine
C_2N	12.8	0.3	
C_3N	14.3	0.3	
C_4N	12.3	0.3	
C_5N	12.0	0.3	
C_6N	12.2	0.3	
C_3HN	11.6	0.3	cynoacetylene
CH_4S	9.44	0.1	

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
Si^-	1.4	0.2
Si	8.151	
Si_2	7.3	0.3
SiH	8.5	0.5
SiH_4	12.2	0.3
SiO	10.51	0.1
SiO_2	11.7	0.5
Si_2O_2	10.	1.0
SiF	7.26	0.1
SiF_2		
SiF_3		
SiF_4	15.4	0.4
Si_2F_4		
SiCl		
$SiCl_2$	11.8	0.4
$SiCl_3$		
$SiCl_4$	12.0	0.4
SiC	9.0	0.3
SiC_2	10.2	0.3
Si_2C	9.1	0.3

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.	
B^-	0.3	0.1	
B	8.298		
B_2	12.4	0.3	
BH	10.0	0.3	
BH_2	8.12	0.3	
BH_3	11.0	1.0	
BO	(7)	1.0	Theoretical estimate
B_2O_2	13.3	0.4	
B_2O_3	13.2	0.4	
HBO_2	12.6	0.4	
BF			
BF_2	9.4	0.4	
BF_3	15.6	0.4	
BF_3^-	2.17	0.4	
BCl	10.44	0.4	
BCl_2	7.20	0.5	
BCl_3	11.5	0.5	
BOF			
BN			
B_2H	10.62	0.5	
B_2H_6	12.0	0.3	
BOCl			

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
BC	10.5	0.3
BC_2	10.7	0.3
B_2C	10.7	0.3
BSi	7.8	0.3
BCSi	9.9	0.3
Al^-	0.5	0.1
Al	5.986	
AlH		
AlO	9.5	0.5
Al_2O	7.7	0.4
Al_2O_2	9.9	0.4
AlO_2H		
AlOF		
AlF	9.5	0.5
AlF_2		
AlF_3		
AlCl		
$AlCl_2$		
$AlCl_3$	12.8	0.8
$AlBr_3$	12.2	0.8

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.	
Be^-	(≤0.1)	0.1	Estimate
Be	9.322		
BeH	8.6		
BeOH			
BeO	6.0	0.5	
$(BeO)_2$			
$(BeO)_3$			
$(BeO)_4$			
$(BeO)_5$			
$(BeO)_6$			
BeF			
BeF_2			
BeCl			
$BeCl_2$			
Mg^-	(≤ 0.1)	0.1	Estimate
Mg	7.646		
MgH			
MgO	8.6	0.5	
MgF			
MgF_2			
MgCl			
$MgCl_2$			

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
Li^-	0.7	0.2
Li	5.392	
Li_2	4.96	0.2
LiH	6.5	0.5
LiO	9.0	0.4
Li_2O	6.8	0.4
LiI	8.55	0.4
Na^-	0.6	0.2
Na	5.139	
Na_2	4.87	0.2
NaH	6.5	1.
NaO	7.6	1.
NaOH	9.0	1.
NaI	8.8	0.4
NaN_3	11.7	0.4